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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) Abstract: Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.

DRUG THERAPY FOR CELIAC SPRUE

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

BACKGROUND OF THE INVENTION

In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

[DQ(a1*03, b1*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a glutenfree diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

SUMMARY OF THE INVENTION

[09] In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10] In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier. In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions. In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

[12] In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

[13]

Methods and compositions are provided for modeling the structure of a soluble (extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding. In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure. The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis. Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor. This information provides a basis for rational drug design.

[14] These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

DETAILED DESCRIPTION OF THE EMBODIMENTS

Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor. Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission. The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions. In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

[17]

Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition. The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention. Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important. Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia. Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

[20]

An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

Among gluten proteins with potential harmful effect to Celiac Sprue patients are [22] included the storage proteins of wheat, species of which include Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskyi; etc. A review of the genes encoding wheat storage proteins may be found in Colot (1990) Genet Eng (N Y) 12:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of α - and γ -gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24] Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as β -alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g., α -methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

[25] The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPPP, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, *inter alia*, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, e.g. by increasing steric hindrance, altering hydrophilicity or hydrophobicity, etc. Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, e.g. by incorporating amino acids known to interact strongly with the binding cleft.

One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

[29] Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX₁ELX₂Y, where X₁ and X₂ are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X₁ and X₂ is a residue other than proline.

Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

[31] The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, e.g. as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, etc. The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35] Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones et al. (1991) Acta Cryst. A47:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger et al. (1998) Acta Cryst. D54:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack et al. (1997) Folding & Design 2:27-42.

[36] It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

[39] It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41] The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moieties.

Computer-based methods of analysis fall into two broad classes: database methods [42] and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g. data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atomby-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[43] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker et al. (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell et al., (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolla, Calif.); and DOCK (Kuntz et al. (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al. (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified. In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage. A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized *de novo*. The *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50] The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, e.g. by the addition of metal ions such as Mn²⁺, Pb²⁺, etc. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, e.g. by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

[54] Alternative methods may also be used. For example, crystals can be characterized by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

[55] Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique. Model building is facilitated by the use of sequence markers, especially selenomethionine residues. Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288). Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones et al., supra.) Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493). Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process. The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

[56] HLA-DQ2/peptide complex structure models and databases of structure information are provided. The structural models find use in determining the structure of related and/or analogous peptide complexes. In some cases, modeling will be based on the provided structure. In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

The structure model may be implemented in hardware or software, or a combination of both. For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape. This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above. Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

[59] Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium. Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[61] Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

[65] For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, corn starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz et al. (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh et al. (2001) J Control Release 71(3):307-18.

[68] Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

[69] The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

METHODS OF TREATMENT

The subject methods are used to treat individuals suffering from Celiac Sprue and/or dematitis herpetiformis, by administering an effective dose through a pharmaceutical formulation. Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art. A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease. Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] are indicative of a susceptibility to the disease. Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity. Methods for the delivery of peptides that are altered from a native peptide are known in the art. Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests. Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

Various methods for administration may be employed. The dosage of the therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like. Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor. A typical dose is at least about 1 μg, usually at least about 10 μg, more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue. Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration. The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, etc. to maintain an effective dosage level.

The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM). IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk. Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, e.g. i.v., i.m., etc. Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

EXPERIMENTAL

Example

[75] It has long been known that the principal toxic components of wheat gluten are a family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α-gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with submicromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant α2-gliadin: α2-gliadin, a representative α-gliadin (Arentz-Hansen et al. (2000) Gut 46:46), was expressed in recombinant form and purified from E. coli. The α2-gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μg/ml of

kanamycin at 37 °C until the OD600 0.6-1 was achieved. The expression of α2-gliadin protein was induced with the addition of 0.4 mM isopropyl α -D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant α2-gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT: 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing α2-gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and α 2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing α 2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min, rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α-2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reversephase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLCgrade acetonitrile/isopropanol: 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30-100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

	33-mer	Control A	Control B
H1P0	<20%	>90%	>90%
H2P0	<20%	>61%	>85%
H3P0	<20%	>87%	>95%
H4P0	<20%	>96%	>95%
H5P0	<20%	>96%	>95%

The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α2-gliadin,

To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of α2 gliadin was then examined. As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity). In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

[79]

Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells. It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α-gliadin

Structural characteristics of the 33-mer gliadin peptide and its naturally occurring [81] homologs: Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire α 2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer a2-gliadin peptide are OPOPFPPOLPYPOTOPFPPOQPYPQPQPQYPQPQ (from α 1- and α 6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from γ-gliadin); VQWPQQQPVPQPHQPF (from γ -gliadin), VQGQGIIQPQQPAQ (from γ -gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from γ-gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from γ-gliadin), QPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from ω -secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins. Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function. In both cases available information suggested that the homology could have biologically relevance. For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein. In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi. In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

Example 3

[83] X-ray Crystallographic Analysis of soluble HLA-DQ2. The soluble extracellular domains of the α - and β -chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered α - and β -chains is provided in SEQ ID NO:1 and SEQ ID NO:2. The β -chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end. Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends. Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

[84]

Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column. Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2 μ L of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2 μ L of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature. Small crystals appeared within three days and grew to full size in two weeks.

[85] For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen. X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using σ_A -weighted F_o - F_c and $2F_o$ - F_c electron density maps with the program O. The current model has R-factor of 0.2209 with a $R_{\rm free}$ of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex, α -chain of DQ2, β -chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex, α -chain, β -chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

Structure-based design of DQ2 binding peptide inhibitors. The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

The coordinate of the structure are as follows:

[89]

[90]

Coordinates

REMARK peptide link removed (applied DPEP): from B 105 to B 113
REMARK peptide link removed (applied DPEP): from E 104 to E 113
REMARK disulphide added: from A 107 to A 163
REMARK disulphide added: from B 15 to B 79
REMARK disulphide added: from B 117 to B 173

REMARK	disulp	hide	add	ed:	from	D	107	to D	163			
REMARK	-						15	to E	79 172			
REMARK REMARK	_				rrom 3:00:6		117 'c	to E reated by	173 v user:	kim		
REMARK				_		-	•		,			
ATOM	1	CB	VAL		2		31.060	3.851	4.095		39.43	A
ATOM	2		VAL		2		30.078	2.835	3.531		40.06	A A
ATOM ATOM	3 4	CG2	VAL VAL		2 2		30.370 30.653	5.185 3.406	4.344 6.542		36.80	A
ATOM	5	ō	VAL		2		29.644	2.702	6.527		38.25	A
MOTA	6	N	VAL		2		32.189	1.926	5.235		36.80	A
MOTA	7	CA	VAL		2		31.684	3.321	5.414		37.95	A
ATOM	8	N	ALA		3		30.910	4.267	7.523		34.99	A
MOTA MOTA	9 10	CA CB	ALA ALA		3 3		30.003	4.416 3.368	8.658 9.721		32.94 33.34	A A
MOTA	11	c	ALA		3		30.094	5.805	9.263		30.81	A
ATOM	12	0	ALA		3		30.980	6.583	8.914	1.00	29.57	A
MOTA	13	N	ASP		4		29.172	6.115	10.170		28.70	A
ATOM	14	CA	ASP		4		29.173	7.416	10.822 11.456		26.95 28.65	A A
MOTA MOTA	15 16	CB CG	ASP ASP		4		27.812 26.687	7.722 7.845	10.431		31.67	A
MOTA	17		ASP		4		26.904	8.417	9.339		33.31	A
ATOM	18	OD2	ASP	A	4		25.568	7.381	10.735	1.00	33.31	A
MOTA	19	C	ASP		4		30.254	7.432	11.898		26.51	A
MOTA	20	0	ASP		4		30.857	8.469	12.170		25.25	A A
ATOM ATOM	21 22	N CA	HIS HIS		5 5		30.493 31.527	6.277 6.164	12.515 13.544		26.22 26.52	A
ATOM	23	CB	HIS		5		30.939	6.339	14.950		25.34	A
ATOM	24	CG	HIS	A	5		30.240	7.647	15.156	1.00	28.69	A
MOTA	25		HIS		5		30.716	8.870	15.492		29.15	A
ATOM	26		HIS		5		28.881	7.801	14.979		28.23 29.92	A A
ATOM ATOM	27 28		HIS		5 5		28.550 29.645	9.062 9.732	15.198 15.511		29.84	A
ATOM	29	C	HIS		5		32.246	4.826	13.465		25.79	A
ATOM	30	0	HIS		5		31.630	3.785	13.227	1.00	25.68	A
MOTA	31	N	VAL		6		33.559	4.866	13.659		24.52	A
ATOM	32	CA	VAL		6 6		34.385	3.667 3.657	13.628 12.407		23.27 25.22	A A
MOTA MOTA	33 34	CB	VAL VAL		6		35.311 36.187	2.414	12.440		24.31	A
ATOM	35		VAL		6		34.489	3.708	11.127		27.15	A
ATOM	36	С	VAL	A	6		35.256	3.633	14.876		22.15	A
ATOM	37	0	VAL		6		35.937	4.606	15.185		21.49	A
ATOM	38 39	N CA	ALA ALA		7 7		35.239 36.038	2.513 2.382	15.586 16.799		19.90 19.70	A A
MOTA MOTA	40	CB	ALA		7		35.132	2.394	18.034		14.59	A
ATOM	41	c	ALA		7		36.867	1.111	16.791		18.62	A
ATOM	42	0	ALA		7		36.548	0.153	16.088		20.78	A
ATOM	43	N	SER		8		37.947	1.120	17.560		16.95	A
ATOM ATOM	44 45	CA CB	SER SER		8 8		38.807 40.211	-0.048 0.215	17.700 17.153		18.62 17.69	A A
ATOM	46	OG	SER		8		40.209	0.271	15,738		19.81	A
MOTA	47	C	SER		8		38.868	-0.310	19.199		18.76	A
MOTA	48	0	SER		8		39.570	0.376	19.943		19.35	A
MOTA	49	N	TYR		9		38.070	-1.268 -1.608	19.645 21.048		19.38 19.44	A A
MOTA MOTA	50 51	CA CB	TYR TYR		9 9		38.038 36.628	-1.980	21.471		19.18	A
ATOM	52	CG	TYR		9		35.714	-0.785	21.375		18.65	A.
MOTA	53		TYR	A	9		36.073	0.435	21.962		16.57	A
MOTA	54		TYR		9		35.237	1.537	21.897		17.39	A
ATOM ATOM	55 E.C		TYR		9		34.493 33.641	-0.865 0.235	20.716 20.647		17.15 16.82	A A
ATOM	56 57	CZ	TYR TYR		9 9		34.020	1.431	21.243		18.07	A
ATOM	58	OH	TYR		9		33.169	2.509	21.210		19.77	A
MOTA	59	C	TYR	A	9		38.993	-2.751	21.106		20.21	A
ATOM	60	0	TYR		9		38.652	-3.911	21.344		15.05	A A
MOTA MOTA	61 62	n Ca	GLY GLY		10 10		40.225 41.311	-2.357 -3.275	20.831		21.69 22.54	A A
ATOM	62 63	CAL	GLY		10		42.276	-3.275	19.655		21.74	A
ATOM	64	ŏ	GLY		10		42.248	-3.863	18.713	1.00	22.02	A
ATOM	65	N	VAL	A	11		43.083	-2.023	19.674		18.91	A
MOTA	66	CA	VAL		11		44.119	-1.949	18.651		17.39 18.75	A A
MOTA MOTA	67 68	CB CG1	VAL VAL		11 11		44.554 45.845	-0.506 -0.558	18.277 17.455		16.18	A
ATOM	69		VAL		11		43.481	0.165	17.432		15.25	A

ATOM	70	С	VAL A	11	45.228	-2.644	19.447	1.00 17.05	A
ATOM	71	ō	VAL A	11	45.679	-2.145	20.481	1.00 19.34	A
MOTA	72	N	ASN A	12	45.616	-3.828	19.005	1.00 17.39	A
ATOM	73	CA	ASN A	12	46.643	-4.597	19.693	1.00 17.18	A
MOTA	74	CB	ASN A	12	46.113	-5.994	20.052	1.00 15.04	A
ATOM	75	CG	ASN A	12	44.834	-5.947	20.882	1.00 15.96	A
ATOM	76		ASN A	12	43.780	-5.490	20.417	1.00 18.20	A
ATOM	77		ASN A	12	44.921	-6.420	22.114	1.00 10.46	A
ATOM	78	C	ASN A	12	47.863	-4.739	18.797	1.00 18.90	A
ATOM	79	0	ASN A	12	47.752	-5.162	17.641	1.00 18.80	A
ATOM	80	N	LEU A	13	49.026	-4.403	19.343	1.00 18.60 1.00 19.90	A A
ATOM	81	CA	LEU A	13	50.264 50.695	-4.478 -3.064	18.599 18.217	1.00 23.26	A
ATOM	82 83	CB CG	LEU A	13 13	52.077	-2.881	17.594	1.00 24.86	A
ATOM ATOM	84		LEU A	13	52.085	-3.494	16.201	1.00 26.92	A
ATOM	85		LEU A	13	52.417	-1.402	17.534	1.00 24.75	A
ATOM	86	C	LEU A	13	51.391	-5.165	19.370	1.00 20.37	A
ATOM	87	o	LEU A	13	51.559	-4.953	20.566	1.00 21.11	A
ATOM	88	N	TYR A	14	52.145	-6.004	18.673	1.00 21.04	A
MOTA	89	CA	TYR A	14	53.291	-6.691	19.255	1.00 24.07	A
ATOM	90	CB	TYR A	14	52.909	-8.050	19.844	1.00 27.05	A
ATOM	91	CG	TYR A	14	54.091	-8.729	20.489	1.00 29.27	A
ATOM	92		TYR A	14	54.569	-8.304	21.723	1.00 30.07	A
ATOM	93	CE1		14	55.709	-8.867	22.285	1.00 31.38	A
ATOM	94	CD2		14	54.783	-9.744	19.830	1.00 31.63	A
ATOM	95	CE2		14		-10.314	20.383	1.00 30.29	A A
MOTA	96	CZ	TYR A	14	56.381	-9.868 -10.413	21.609 22.160	1.00 31.37 1.00 34.48	A
ATOM ATOM	97	C OH	TYR A	14 14	54.291	-6.900	18.128	1.00 25.30	A
ATOM	98 99	0	TYR A	14	53.907	-7.206	16.994	1.00 25.51	A
MOTA	100	N	GLN A	15	55.571	-6.725	18.429	1.00 24.61	A
ATOM	101	CA	GLN A	15	56.603	-6.891	17.414	1.00 25.19	A
ATOM	102	СВ	GLN A	15	56.932	-5.549	16.754	1.00 23.54	A
ATOM	103	CG	GLN A	15	57.278	-4.443	17.738	1.00 23.98	A
ATOM	104	CD	GLN A	15	57.567	-3.116	17.056	1.00 26.32	A
MOTA	105	OE1	GLN A	15	57.575	-2.062	17.702	1.00 28.26	A
MOTA	106	NE2	GLN A	15	57.810	-3.159	15.749	1.00 24.64	A
ATOM	107	C	GLN A	15	57.848	-7.487	18.036	1.00 26.16	A
MOTA	108	0	GLN A	15	58.134	-7.263	19.211	1.00 24.31	A
MOTA	109	N	SER A	16	58.583	-8.252	17.236	1.00 28.72	A
MOTA	110	CA	SER A	16	59.801	-8.912	17.698	1.00 30.37	A A
MOTA	111	CB	SER A	16	60.341	-9.830 -9.100	16.603	1.00 28.35 1.00 31.43	A
MOTA	112	OG	SER A	16	60.569 60.883	-7.918	15.407 18.111	1.00 32.37	A
MOTA MOTA	113 114	C O	SER A SER A	16 16	61.538	-8.104	19.134	1.00 33.91	A
ATOM	115	И	TYR A	17	61.073	-6.863	17.325	1.00 32.49	A
ATOM	116	CA	TYR A	17	62.096	-5.890	17.664	1.00 34.27	A
ATOM	117	СВ	TYR A	17	62.172	-4.788	16.620	1.00 35.41	A
ATOM	118	CG	TYR A	17	63.371	-3.911	16.837	1.00 37.77	A
MOTA	119	CD1	TYR A	17	64.646	-4.347	16.470	1.00 39.38	A
MOTA	120	CEI	L TYR A	17	65.769	-3.569	16.715	1.00 40.15	A
MOTA	121	CD2		17	63.247	-2.671	17.456	1.00 36.31	A
MOTA	122	CE2		17	64.360	-1.886	17.707	1.00 39.40	A A
MOTA	123	CZ	TYR A	17	65.621	-2.338	17.335	1.00 41.42 1.00 43.02	A
ATOM	124	OH	TYR A	17	66.732 61.821	-1.562 -5.270	17.580 19.027	1.00 34.43	A
ATOM	125	C	TYR A		60.765	-4.682	19.248	1.00 35.58	A
MOTA MOTA	126 127	Ŋ	TYR A		62.783	-5.390	19.935	1.00 34.98	A
ATOM	128	CA	GLY A		62.609	-4.854	21,270	1.00 35.78	A
ATOM	129	c	GLY A		62.730	-5.968	22,292	1.00 36.87	A
ATOM	130	ō	GLY A		63.761	-6.082	22.952	1.00 38.48	A
MOTA	131	N	PRO A		61.692	-6.807	22.459	1.00 37.06	A
ATOM	132	CD	PRO A	19	61.745	-7.967	23.368	1.00 35.58	A
MOTA	133	CA	PRO A		60.409	-6.769	21.747	1.00 34.79	A
MOTA	134	CB	PRO A		59.853	-8.166	21.981	1.00 35.91	A
MOTA	135	CG	PRO A		60.300	-8.437	23.394	1.00 36.88	A
MOTA	136		PRO A	_	59.531	-5.706	22.379	1.00 33.10 1.00 33.71	A A
ATOM	137		PRO A		59.844 58.435	-5.209 -5.349	23.456 21.722	1.00 33.71	A
MOTA	138		SER A		57.548	-4.341	22.290	1.00 30.25	A
ATOM	139		SER A		58.060		21.965	1.00 29.00	A.
ATOM ATOM	140 141				58.072		20.567	1.00 32.27	A
ATOM	142		SER A		56.108			1.00 27.93	A
ATOM	143		SER A		55.829			1.00 28.23	A

			GLY	24	21	55.191	-3.911	22.576	1.00 25.87	A
MOTA	144	N			21	53.797		.22.222	1.00 23.78	A
ATOM	145	CA	GLY		21	53.076	-2.732	22.598	1.00 23.94	A
ATOM	146	C	GLY			53.638	-1.840	23.247	1.00 24.81	A
ATOM	147	0	GLY		21		-2.641	22.187	1.00 20.60	A
MOTA	148	N	GTN		22	51.821			1.00 19.67	A
ATOM	149	CA	GLN		22	51.033	-1.470	22.495		A
MOTA	150	CB	GLN		22	51.239	-0.400	21.415	1.00 19.28	
MOTA	151	CG	GLN	A	22	50.584	0.943	21.736	1.00 18.12	A
MOTA	152	CD	GLW	A	22	50.732	1.971	20.613	1.00 18.84	A
MOTA	153	OE1	GLN	A	22	51.694	2.749	20.576	1.00 19.77	A
ATOM	154	NE2	GLN	A	22	49.777	1.968	19.688	1.00 16.83	A
MOTA	155	C	GLN		22	49.573	-1.873	22.566	1.00 18.66	A
MOTA	156	ō	GLN		22	49.128	-2.747	21.826	1.00 18.45	A
			TYR		23	48.842	-1.257	23.484	1.00 17.25	A
MOTA	157	N				47.423	-1.529	23.615	1.00 16.53	A
MOTA	158	CA	TYR		23		-2.497	24.752	1.00 14.51	A
MOTA	159	CB	TYR		23	47.127			1.00 12.67	A
ATOM	160	CG	TYR		23	45.674	-2.904	24.760	1.00 13.38	A
ATOM	161		TYR		23	45.251	-4.070	24.121		
ATOM	162	CE1	TYR	A	23	43.904	-4.415	24.070	1.00 13.23	A
ATOM	163	CD2	TYR	A	23	44.713	-2.093	25.346	1.00 11.07	A
ATOM	164	CE2	TYR	A	23	43.365	-2.425	25.299	1.00 12.99	A
ATOM	165	CZ	TYR	A	23	42.964	-3.583	24.664	1.00 13.72	A
ATOM	166	OH	TYR	. A	23	41.624	-3.907	24.611	1.00 17.15	A
ATOM	167	c	TYR		23	46.694	-0.220	23.860	1.00 16.88	A
	168	ō	TYR		23	46.975	0.491	24.824	1.00 16.57	A
ATOM			THR		24	45.757	0.085	22.969	1.00 16.16	A
MOTA	169	N			24	44.975	1.311	23.038	1.00 16.43	A
ATOM	170	CA	THE			45.594	2.405	22.136	1.00 18.41	A
MOTA	171	CB	THE		24		1.954	20.771	1.00 17.20	A
ATOM	172		THE		24	45.581			1.00 18.64	A
MOTA	173	CG2			24	47.029	2.692	22.537		A
MOTA	174	C	THE	A	24	43.570	1.058	22.499	1.00 15.15	
ATOM	175	0	THE	ΑJ	24	43.314	0.037	21.879	1.00 15.70	A
ATOM	176	N	HIS	A	25	42.667	1.993	22.754	1.00 15.66	A
ATOM	177	CA	HIS	A	25	41.320	1.924	22.210	1.00 15.79	A
ATOM	178	СВ	HIS	A	25	40.243	1.834	23.297	1.00 13.55	A
ATOM	179	CG	HIS		25	39.956	0.430	23.734	1.00 15.91	A
ATOM	180		HIS		25	40.688	-0.704	23.624	1.00 13.86	A
			HIS		25	38.790	0.071	24.374	1.00 15.91	A
MOTA	181				25	38.815	-1.222	24.639	1.00 14.38	A
MOTA	182		HIS			39.956	-1.715	24.193	1.00 16.99	A
ATOM	183		HI		25		3.212	21.437	1.00 14.18	A
ATOM	184	C		S A	25	41.176		21.865	1.00 13.52	A
MOTA	185	0		S A	25	41.677	4.241		1.00 14.81	A
ATOM	186	N		JA	26	40.510	3.150	20.292		A
MOTA	187	CA	GT!	IJΑ	26	40.333	4.329	19.462	1.00 16.96	
ATOM	188	CB		σA	26	41.132	4.188	18.164	1.00 16.34	A
ATOM	189	CG	GL	UΑ	26	42.644	4.158	18.311	1.00 18.80	A
ATOM	190	CD	GL	UΑ	26	43.345	4.036	16.958	1.00 22.68	, A
ATOM	191	OE:	L GL	ŲΑ	26	42.744	4.456	15.946	1.00 26.77	A
ATOM	192	OE:	2 GL	υA	26	44.490	3.539	16.901	1.00 20.46	A
ATOM	193	C	GL	U A	26	38.875	4.543	19.101	1.00 17.22	A
ATOM	194	ō		U A	26	38.104	3.597	18.996	1.00 18.66	A
	195	N		ΕA	27	38.503	5.802	18.917	1.00 18.91	A
MOTA	196			ΕA		37,150	6.135		1.00 19.32	A
ATOM				ΕA		36.290	6.546		1.00 20.19	A
MOTA	197			E A		34.834				A
MOTA	198		1 PH			34.024				A
MOTA	199									A
MOTA	200		2 PH			34.289				A
MOTA	201		1 PH			32.692				A
MOTA	202	CE	2 PH			32.954				A
MOTA	203	CZ	PH	Œ A		32.155				
MOTA	204	C	PH	ŒA	. 27	37.260	7.291			A
ATOM	205	0	PE	Œ A	. 27	37.733	8.375			A
MOTA	206			P A		36.831	7.052			A
ATOM	207			P P		36.901	8.060	15.227		A
MOTA	208			3P }		35.910			1.00 21.33	A
	209			3P #		34.472				A
MOTA			1 AS			34.26				A
MOTA	210		2 AS	2D 7	28	33.552				A
ATOM	211			SP 1		38.29				A
ATOM	212			3P /		38.46				A
MOTA	213					39.29				A
MOTA	214			LY						A
ATOM	21			LY J		40.65				A
ATOM	210			LY X		41.43				A
MOTA	21	7 0	G)	LY Z	A 29	42.62	1 9.01	0 15.814	1.00 49.20	•

ATOM	218	N	ASP	A	30	40.797	8.922	17.098	1.00 16.92	A
ATOM	219	CA	ASP		30	41.511	9.438	18.254	1.00 16.83	A
MOTA	220	CB	ASP		30	40.816	10.678	18.796	1.00 18.99	A
MOTA	221	CG	ASP		30	40.988 42.145	11.864 12.177	17.888 17.538	1.00 21.09 1.00 22.94	A A
ATOM ATOM	222 223		ASP ASP		30 30	39.971	12.478	17.525	1.00 21.68	A
ATOM	224	C	ASP		30	41.656	8.392	19.345	1.00 17.25	A
ATOM	225	ō	ASP		30	40.777	7.553	19.543	1.00 15.40	A
ATOM	226	N	GLU		31	42.784	8.453	20.041	1.00 16.77	A
ATOM	227	CA	GLU	A	31	43.111	7.514	21.107	1.00 18.43	A
MOTA	228	CB	GLU	A	31	44.620	7.607	21.392	1.00 20.90	A
MOTA	229	CG	GLU		31	45.147	6.853	22.608	1.00 24.68	A
ATOM	230	CD	GLU		31	46.678 47.258	6.924 7.931	22.702 22.239	1.00 27.25 1.00 26.93	A A
ATOM ATOM	231 232		GLU		31 31	47.230	5.985	23.242	1.00 27.21	A
ATOM	233	C	GLU		31	42.296	7.777	22.375	1.00 17.51	A
ATOM	234	ō	GLU		31	42.361	8.863	22.952	1.00 17.13	A
MOTA	235	N	GLN	A	32	41.525	6.784	22.807	1.00 15.52	A
MOTA	236	CA	GLN	A	32	40.726	6.942	24.020	1.00 16.47	A
ATOM	237	CB	GLN		32	39.542	5.980	24.009	1.00 15.91	A
ATOM	238	CG	GLN		32	38.439	6.399	23.065 23.071	1.00 15.97 1.00 20.20	A A
MOTA	239	CD	GLN GLN		32 32	37.292 37.478	5.419 4.228	22.808	1.00 18.09	A
ATOM ATOM	240 241		GLN		32	36.091	5.912	23.374	1.00 20.57	A
MOTA	242	C	GLN		32	41.584	6.701	25.255	1.00 16.61	A
ATOM	243	ō	GLN		32	41.448	7.387	26.272	1.00 15.51	A
ATOM	244	N	PHE	A	33	42.470	5.720	25.151	1.00 15.59	A
ATOM	245	CA	PHE		33	43.370	5.389	26.239	1.00 16.34	A
ATOM	246	CB	PHE		33	42.583	4.854	27.443 27.222	1.00 17.21 1.00 16.68	A A
ATOM	247	CG	PHE		33 33	41.951 42.686	3.502 2.333	27.406	1.00 15.57	A
MOTA MOTA	248 249		PHE		33	40.598	3.397	26.903	1.00 18.54	A
ATOM	250		PHE		33	42.083	1.076	27.288	1.00 16.34	A
ATOM	251		PHE		33	39.983	2.147	26.782	1.00 17.35	A
MOTA	252	\mathbf{cz}	PHE	A	33	40.729	0.983	26.978	1.00 16.56	A
MOTA	253	C	PHE		33	44.363	4.343	25.776	1.00 16.66	A
ATOM	254	0	PHE		33	44.209	3.746	24.712	1.00 16.85 1.00 16.03	A A
MOTA	255	N	TYF		34 34	45.398 46.377	4.139 3.125	26.572 26.264	1.00 16.03	A
ATOM ATOM	256 257	CA CB	TYF		34	47.636	3.730	25.621	1.00 16.33	A
ATOM	258	CG	TYF		34	48.528	4.541	26.523	1.00 17.31	A
ATOM	259		TYF		34	49.519	3.930	27.291	1.00 17.48	A
ATOM	260	CE1	TYP	A S	34	50.367	4.683	28.097	1.00 19.16	A
ATOM	261		TYF		34	48.404	5.928	26.586	1.00 17.68	A
MOTA	262	CE2			34	49.244	6.690	27.388 28.141	1.00 19.73 1.00 20.10	A A
ATOM	263	CZ	TYI	AS	34 34	50.224 51.044	6.060 6.815	28.941	1.00 23.02	A
ATOM ATOM	264 265	C		R S	34	46.692	2.473	27.588	1.00 17.88	A
ATOM	266	ō	TY		34	46.429	3.042	28.646	1.00 21.13	A
MOTA	267	N	VAI		35	47.213	1.261	27.535	1.00 17.31	A
MOTA	268	CA	VAI	L A	35	47.571	0.570	28.749	1.00 18.89	A
MOTA	269	CB		ЬA	35	46.950	-0.848	28.804	1.00 19.12	A
ATOM	270		L VA		35	47.589	-1.660 -0.742	29.912 29.048	1.00 17.56 1.00 19.75	A A
MOTA	271	CG2	VAI	ЬA		45.454 49.084	0.478	28.786	1.00 18.84	A
MOTA MOTA	272 273	o		LΑ		49.701	-0.050	27.877	1.00 16.51	A
MOTA	274	N		PΑ		49.676	1.039	29.830	1.00 22.55	A
MOTA	275	CA	AS:	P A	. 36	51.121	0.984	29.996	1.00 25.86	A
MOTA	276	CB		P A		51.542	1.872	31.172	1.00 26.89	A
MOTA	277	CG		PA		53.033	2.108	31.221 31.270	1.00 26.55 1.00 29.78	A A
MOTA	278		LAS			53.796 53.441	1.125 3.285		1.00 30.03	A
MOTA	279 280	C C	2 AS	P A		51.393	-0.484		1.00 26.39	A
MOTA MOTA	281	Ö		P A		51.016	-0.976	31.378	1.00 27.38	A
ATOM	282			UΑ		52.024	-1.187	29.387		A
MOTA	283			U A		52.305	-2.600		1.00 29.51	A
MOTA	284			U A		52.754				A
MOTA	285			U A		51.704				A A
MOTA	286		2 LE			52.265 50.455				A
ATOM ATOM	287 288			UA		53.348				A
MOTA	289			UA		53.222				A
ATOM	290		GL	Y P	38	54.362	-1.980			A
MOTA	291		GI	Y P	38	55.403	-2.140	31.737	1.00 35.44	A

ATOM	292	С	GLY	Δ	38	54.956	-1.863	33.162	1.00 37.63	A
MOTA	293	ō	GLY		38	55.369	-2.549	34.098	1.00 38.42	A
ATOM	294	N	ARG		39	54.101	-0.861	33.334	1.00 38.93	A
ATOM	295	CA	ARG		39	53.625	-0.499	34.660	1.00 40.81	A
ATOM	296	СВ	ARG		39	53.645	1.029	34.803	1.00 42.41	A
ATOM	297	CG	ARG		39	54.968	1.627	34.339	1.00 44.76	A
ATOM	298	CD	ARG	A	39	55.113	3.118	34.619	1.00 47.83	A
ATOM	299	NE	ARG	A	39	56.318	3.644	33.976	1.00 50.52	A
ATOM	300	CZ	ARG	A	39	56.902	4.799	34.281	1.00 53.40	A
ATOM	301	NH1	ARG	A	39	56.399	5.575	35.235	1.00 54.01	A
MOTA	302	NH2	ARG	A	39	57.998	5.179	33.633	1.00 54.18	A
ATOM	303	С	ARG	A	39	52.229	-1.057	34.936	1.00 41.12	A
MOTA	304	0	ARG	A	39	51.664	-0.847	36.014	1.00 39.71	A
MOTA	305	N	LYS	A	40	51.687	-1.779	33.955	1.00 40.65	A
ATOM	306	CA	LYS	A	40	50.365	-2.380	34.070	1.00 39.55	A
MOTA	307	CB	LYS	A	40	50.415	-3.554	35.053	1.00 42.42	A
ATOM	308	CG	LYS	A	40	49.196	-4.467	34.996	1.00 46.46	A
ATOM	309	СD	LYS	A	40	49.266	-5.563	36.054	1.00 50.42	A
MOTA	310	CE	LYS	A	40	48.077	-6.513	35.947	1.00 51.25	A
MOTA	311	NZ	LYS		40	46.781	-5.779	35.970	1.00 52.15	A
MOTA	312	C	LYS		40	49.338	-1.348	34.540	1.00 37.45	A
MOTA	313	0	LYS		40	48.647	-1.560	35.533	1.00 35.78	A A
MOTA	314	N	GLU		41	49.245	-0.237	33.812	1.00 35.81	A
MOTA	315	CA	GLU		41	48.317	0.847	34.142	1.00 33.83 1.00 36.46	A
MOTA	316	CB	GLU		41	49.077	2.079	34.655	1.00 41.33	A
MOTA	317	CG	GLU		41	49.660	1.997	36.049 36.374	1.00 44.23	A
MOTA	318	CD	GLU		41	50.500	3.224	36.022	1.00 46.67	A
MOTA	319		GLU		41	50.067	4.343	36.981	1.00 45.55	A
MOTA	320		GLU		41	51.585 47.492	1.301	32.937	1.00 30.89	A
MOTA	321	C	GLU		41 41	47.995	1.373	31.816	1.00 27.89	A
ATOM ATOM	322	Ŋ	THE		42	46.227	1.623	33.182	1.00 28.11	A
ATOM	323 324	CA	THE		42	45.354	2.127	32.135	1.00 26.58	A
ATOM	325	CB	THE		42	43.882	1.773	32.406	1.00 27.67	A
MOTA	326		THE		42	43.716	0.349	32.394	1.00 25.55	A
MOTA	327	CG2			42	42.979	2.419	31.357	1.00 25.33	A
ATOM	328	C	THE		42	45.506	3.642	32.212	1.00 26.90	A
ATOM	329	ō	THE		42	45.305	4.232	33.269	1.00 25.79	A
ATOM	330	N	VAI		43	45.881	4.273	31.108	1.00 25.87	A
ATOM	331	CA	VAI	A	43	46.045	5.720	31.106	1.00 24.36	A
ATOM	332	CB	VAI	A	43	47.474	6.119	30.670	1.00 24.45	A
MOTA	333	CG1	. VAI	A	43	47.698	7.606	30.906	1.00 24.38	A
MOTA	334	CG2	VAI	LΑ	43	48.504	5.289	31.433	1.00 22.82	A
ATOM	335	C	VAI	LΑ	43	45.039	6.331	30.141	1.00 24.94	A
MOTA	336	0	VAI	LΑ	43	45.143	6.133	28.930	1.00 24.72	A
MOTA	337	N	TRI	PΑ	44	44.063	7.065	30.672	1.00 24.50	A
MOTA	338	CA	TRI	PΑ	44	43.050	7.681	29.824	1.00 25.64	A
MOTA	339	CB		PΑ	44	41.804	8.033	30.642	1.00 25.03	A
ATOM	340	CG		PΑ	44	41.224	6.859	31.370	1.00 25.96 1.00 25.77	A A
MOTA	341		2 TRI		44	40.281	5.906	30.858	1.00 25.77	A
MOTA	342		2 TR		44	40.067	4.946	31.870 29.641	1.00 24.94	A
ATOM	343	CE		PA	44	39.599	5.766	32.634	1.00 26.43	A
MOTA	344		L TR			41.529 40.840	6.450 5.305	32.942	1.00 26.28	A
MOTA	345		1 TR			39.197	3.860	31.704	1.00 25.00	A
MOTA	346		2 TR			38.734	4.688	29.476	1.00 22.40	A
MOTA	347		2 TR			38.542	3.749		1.00 24.18	A
MOTA MOTA	348 349			PΑ		43.578	8.925	_	1.00 26.30	A
ATOM	350			PΑ		44.321	9.713		1.00 24.42	A
MOTA	351			SA		43.193			1.00 28.01	A
ATOM	352			SA		43.635			1.00 30.22	A
MOTA	353			SA		44.069			1.00 29.51	A
MOTA	354			SA		45.547		25.680	1.00 30.66	A
ATOM	355			SA		42.574		26.951	1.00 31.06	A
MOTA	356			SA		42.836	12.399			A
ATOM	357			U A		41.375				A
MOTA	358		LE	U A		40.261		_		A
MOTA	359			U A		39.137				A
MOTA	360			U A	46	38.810				A
ATOM	361	CD	1 LE			37.492				A
ATOM	362		2 LE			38.710				A
ATOM	363			U F		39.734				A
ATOM	364	1 0		EU #		39,195				A
ațom	365	5 N	PF	lo I	47	39.893	13.201	29.521	1.00 32.52	A

ATOM 367 CA PRO A 47 39.437 13.392 30.901 1.00 32.18 A ATOM 368 CB PRO A 47 39.487 14.908 31.063 1.00 32.11 A	ATOM	366	CD	PRO	A	47	40.488	14.442	28.986	1.00 32.23	A
XTOM 366 CD PRO A 47 39,487 14,908 31,003 1,00 32,11 A ATOM 370 C PRO A 47 38,066 12,800 31,245 1,00 30,96 A ATOM 371 O PRO A 47 37,927 12,100 31,245 1,00 30,96 A ATOM 372 N VAL 4 88 35,715 12,583 30,663 1,00 30,755 A ATOM 376 CB VAL A 88 34,748 13,040 29,932 1,00 34,04 A AROM 376 CG2 VAL A 88 34,748 13,040 29,260 1,00 34,04 A AROM 376 CG VAL A 34 34,688 13,198 2,10 13,00 36,0 A AROM 380 CA LEDIA 49 36,661 8											A
ATOM 369 CG PRO A 47	ATOM						39.487	14.908	31.063	1.00 32.11	A
ARTON 371 0 PBO A 47 37.927 12.103 32.243 1.00 30.17 A A TROM 372 N VAL A 48 35.715 12.563 30.466 1.00 32.56 A ARTON 373 CN VAL A 48 35.715 12.563 30.663 1.00 32.56 A ARTON 375 CSI VAL A 48 33.120 12.683 29.392 1.00 34.16 A ARTON 376 CSI VAL A 48 33.200 12.683 29.392 1.00 34.16 A ARTON 377 C VAL A 48 33.200 12.683 29.366 1.00 32.56 A ARTON 377 C VAL A 48 33.200 12.683 29.392 1.00 34.16 A ARTON 378 CSI VAL A 48 34.692 14.556 29.366 1.00 33.31 A ARTON 378 N LEUT A 49 36.661 10.455 31.355 1.00 33.55 A ARTON 378 N LEUT A 49 36.661 8.992 30.192 1.00 33.30 A ARTON 378 N LEUT A 49 36.661 8.992 30.208 1.00 33.30 A ARTON 390 CD LEUT A 49 37.783 8.192 12.003 31.00 30.62 A ARTON 392 CD LEUT A 49 37.783 8.157 26.551 1.00 33.164 A ARTON 391 CD LEUT A 49 37.783 8.157 26.551 1.00 31.65 A ARTON 392 CD LEUT A 49 37.783 8.157 26.551 1.00 31.05 A ARTON 396 C LEUT A 49 37.783 8.157 26.551 1.00 31.05 A ARTON 396 C LEUT A 49 37.783 8.157 26.551 1.00 31.05 A ARTON 398 C LEUT A 49 37.783 8.157 26.551 1.00 31.05 A ARTON 396 C ARGA 50 38.367 8.810 33.618 1.00 35.58 A ARTON 398 C ARGA 50 38.367 8.810 33.618 1.00 35.58 A ARTON 398 C ARGA 50 38.367 8.810 33.618 1.00 35.58 A ARTON 398 C ARGA 50 38.367 8.810 33.618 1.00 35.58 A ARTON 399 C ARGA 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 C ARGA 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 37.334 8.168 34.591 1.00 44.85 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.137 10.720 33.636 1.00 40.65 A ARTON 399 N MAR A 50 50 40.13	ATOM	369	CG	PRO	A	47	40.690	15.270			
APON 372 N VIAL A 8 37.066 13.068 30.418 1.00 30.75 A A A A A A A A A	MOTA	370	C								
ARON 372 CA VML A 48 35.715 12.563 30.663 1.00 32.56 A A ARON 375 CG1 VML A 48 31.20 12.683 29.932 1.00 34.16 A ARON 375 CG1 VML A 48 33.20 12.683 29.932 1.00 34.16 A ARON 376 CG2 VML A 48 33.20 12.683 29.932 1.00 34.16 A ARON 377 C VML A 48 33.20 12.683 29.932 1.00 34.16 A ARON 378 CG1 VML A 48 33.20 12.683 29.932 1.00 33.13 A ARON 379 N LEU A 48 33.633 11.033 30.765 1.00 33.31 A ARON 379 N LEU A 49 36.615 10.350 30.195 1.00 33.35 A ARON 379 N LEU A 49 36.615 10.350 30.195 1.00 33.30 A ARON 380 CD LEU A 49 37.698 8.991 29.023 1.00 30.62 A ARON 382 CD LEU A 49 37.698 8.991 29.023 1.00 30.62 A ARON 382 CD LEU A 49 37.783 8.157 26.551 1.00 33.05 A ARON 382 CD LEU A 49 37.783 8.157 26.551 1.00 33.05 A ARON 385 C LEU A 49 37.783 8.157 26.551 1.00 31.05 A ARON 386 C LEU A 49 37.783 8.157 26.551 1.00 31.05 A ARON 386 C LEU A 49 37.783 8.157 26.551 1.00 31.05 A ARON 386 C LEU A 49 37.783 8.157 26.551 1.00 31.05 A ARON 386 C ARON 380 C ARON											
ARTOM 375 CB VAL A 48 34.748 13.040 29.550 1.00 34.04 A A ARTOM 375 CG1 VAL A 48 33.120 12.630 29.932 1.00 34.04 A A ARTOM 376 CG2 VAL A 48 33.120 12.630 29.932 1.00 34.04 A ARTOM 377 C VAL A 48 34.691 14.556 29.366 1.00 38.02 A ARTOM 378 O VAL A 48 34.692 10.485 31.355 1.00 33.355 A ARTOM 378 O VAL A 48 34.692 10.485 31.355 1.00 33.355 A ARTOM 378 O VAL A 48 34.692 10.485 31.355 1.00 33.355 A ARTOM 380 CA LEU A 49 36.612 8.092 30.208 1.00 30.464 A ARTOM 379 N LEU A 49 37.498 8.991 29.023 1.00 30.622 A ARTOM 380 COL LEU A 49 37.498 8.991 29.023 1.00 30.62 A ARTOM 380 CD LEU A 49 37.728 8.888 27.464 1.00 29.12 A ARTOM 383 CD LEU A 49 37.728 8.888 27.464 1.00 29.12 A ARTOM 385 C LEU A 49 37.728 8.888 27.464 1.00 32.144 A ARTOM 385 C LEU A 49 37.7286 8.343 31.519 1.00 33.77 A ARTOM 386 C ARTOM 380 C LEU A 49 37.7286 8.343 31.519 1.00 33.77 A ARTOM 385 C LEU A 49 37.7286 8.343 31.519 1.00 34.56 A ARTOM 389 CB ARTOM 380 CO ARTOM 380											
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ATCOM 377 C C02 VAL A 48 34.881 14.556 29.368 1.00 38.02 A ATCOM 377 C VAL A 48 35.633 11.033 30.765 1.00 33.13 A ATCOM 378 O VAL A 48 34.698 10.485 31.355 1.00 33.55 A ATCOM 379 N LEU A 49 36.615 10.505 0.009 31.355 1.00 33.55 A ATCOM 379 N LEU A 49 36.615 10.505 0.009 31.00 32.44 A ATCOM 379 N LEU A 49 37.498 8.191 29.023 1.00 30.62 A ATCOM 381 CB LEU A 49 37.498 8.191 29.023 1.00 30.62 A ATCOM 382 CG LEU A 49 37.498 8.191 29.023 1.00 30.62 A ATCOM 383 CDL LEU A 49 37.598 8.888 27.464 1.00 29.12 A ATCOM 385 C LEU A 49 37.783 8.157 26.551 1.00 31.05 A ATCOM 385 C LEU A 49 37.226 8.343 31.519 1.00 33.75 A ATCOM 386 C LEU A 49 37.226 8.343 31.519 1.00 33.75 A ATCOM 387 N ARG A 50 37.794 9.221 32.339 1.00 34.14 A ATCOM 387 N ARG A 50 38.367 8.180 33.618 1.00 35.58 A ATCOM 389 C ARG A 50 40.657 11.846 13.03 36.18 1.00 33.55 A ATCOM 389 C ARG A 50 40.657 11.846 13.03 36.18 1.00 35.58 A ATCOM 390 C ARG A 50 40.657 11.846 13.829 1.00 43.05 A ATCOM 391 C ARG A 50 40.657 11.846 13.829 1.00 43.05 A ATCOM 392 N ATCOM 393 C ARG A 50 40.657 11.846 13.829 1.00 43.05 A ATCOM 393 C ARG A 50 40.657 11.846 13.829 1.00 43.05 A ATCOM 394 NHL ARG A 50 40.657 11.846 13.829 1.00 44.05 A ATCOM 395 N ATCOM 396 C ARG A 50 42.854 11.159 33.592 1.00 46.76 A ATCOM 396 C ARG A 50 42.854 11.159 33.592 1.00 46.08 A ATCOM 397 O ARG A 50 43.254 11.159 33.592 1.00 46.08 A ATCOM 398 N BL ARG A 50 43.254 11.159 33.592 1.00 46.08 A ATCOM 396 C ARG A 50 43.254 11.159 33.592 1.00 46.06 A ATCOM 396 C ARG A 50 43.254 11.159 33.592 1.00 46.06 A ATCOM 399 C ARG A 50 43.254 11.159 33.592 1.00 46.08 A ATCOM 399 C ARG A 50 43.254 11.159 33.592 1.00 46.08 A ATCOM 400 C B GLN A 51 33.658 8 .558 34.547 1.00 35.55 A ATCOM 400 C B GLN A 51 33.658 8 .558 34.547 1.00 35.52 A ATCOM 400 C B GLN A 51 33.658 8 .558 34.821 1.00 37.34 A ATCOM 400 C B GLN A 51 33.658 8 .559 34.821 1.00 37.34 A ATCOM 400 C B GLN A 51 33.658 8 .559 34.821 1.00 37.94 A ATCOM 400 C B GLN A 51 33.658 8 .559 34.821 1.00 32.22 A ATCOM 400 C B GLN A 51 33.668 8 .559 34.821 1.00 32.22 A ATCOM 40											
AROM											
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XNOM 379 N LEU A 9 36.615 10.350 30.192 1.00 33.44 A XNOM 381 CB LEU A 9 37.498 8.391 29.023 1.00 32.44 A ARTOM 382 CG LEU A 9 35.678 8.137 29.023 1.00 31.64 A ARTOM 384 CDL LEU A 9 37.783 8.157 26.551 1.00 31.364 A ARTOM 386 O LEU A 9 37.236 8.131 31.787 1.00 33.777 A ARTOM 388 CA ARG 50 37.794 9.21 32.339 1.00 34.555 A ARTOM 390 CG ARG 50 40.571 1.00 33.618 1.00 31.797 9.21 32.339 1.00 43.556 A ARTOM 390 </td <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>34.698</td> <td>10.485</td> <td>31.355</td> <td></td> <td></td>							34.698	10.485	31.355		
ATOM 381 CB LEU A 49 37,488 8,391 29,023 1,00 30,62 A A A A A A A A A		379	N	LEU	A	49	36.615				
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ATOM 438 C PHE A 54 40.597 -1.711 33.017 1.00 23.43 A											
									33.351	1.00 23.53	A

ATOM	440	N	ASP	20	55	40.408	-3.011	33.198	1,00 22.82	A
ATOM	441	CA	ASP		55	41.411	-3.874	33.805	1.00 24.70	A
ATOM	442	CB	ASP		55	40.785	-5.246	34.083	1.00 23.26	A
ATOM	443	CG	ASP		55	41.729	-6.190	34.789	1.00 26.24	A
MOTA	444		ASP		55	42.924	-5.853	34.933	1.00 28.75	A
ATOM	445		ASP		55	41.274	-7.279	35.192	1.00 26.38	A
ATOM	446	C	ASP		55	42.613	-4.011	32.861	1.00 24.24	A
ATOM	447	ŏ	ASP		55	42.510	-4.629	31.802	1.00 23.91	A
ATOM	448	N	PRO		56	43.770	-3.437	33.238	1.00 23.69	A
ATOM	449	CD .	PRO		56	44.084	-2.761	34.509	1.00 23.79	A
ATOM	450	CA	PRO		56	44.961	-3.522	32.387	1,00 23.45	A
ATOM	451	CB	PRO		56	46.002	-2.707	33.162	1,00 23.35	A
ATOM	452	CG	PRO		56	45.592	-2.897	34.580	1.00 23.31	A
ATOM	453	C	PRO	A	56	45.413	-4.952	32.114	1.00 23.66	A
ATOM	454	0	PRO	A	56	46.099	-5.220	31.125	1.00 23.15	A
ATOM	455	N	GLN	A	57	45.025	-5.871	32.991	1.00 21.84	A
ATOM	456	CA	GLN	A	57	45.397	-7.261	32.818	1.00 22.47	A
ATOM	457	CB	GTN	A	57	44.834	-8.108	33.965	1.00 23.11	A
ATOM	458	CG	GLN	A	57	45.226	-9.568	33.873	1.00 20.82	A
MOTA	459	CD	GLN	A	57	46.722	-9.745	33.733	1.00 22.23	A
MOTA	460		GLN		57	47.497	-9.227	34.539	1.00 21.88	A
MOTA	461	NE2	GLN		57	47.138		32.707	1.00 23.15	A
ATOM	462	С	GLN		57	44.882	-7.792	31.482	1.00 22.21	A A
MOTA	463	0	GLN		57	45.452	-8.723	30.913	1.00 23.00	A
ATOM	464	N	PHE		58	43.801	-7.203	30.980	1.00 22.42 1.00 21.07	A
ATOM	465	CA	PHE		58	43.254	-7.640	29.704 29.338	1.00 20.45	A
ATOM	466	CB	PHE		58	42.004	-6.857 -7.287	28.031	1.00 20.43	A
MOTA	467	CG	PHE		58	41.411 40.472	-8.312	27.988	1.00 18.42	A
ATOM	468		PHE PHE		58	41.864	-6.736	26.835	1.00 18.79	A
ATOM	469		PHE		58 58	39.992	-8.792	26.765	1.00 21.25	A
ATOM	470 471		PHE		58	41.393	-7.207	25.610	1.00 20.28	A
MOTA MOTA	472	CZ	PHE		58	40.457	-8.238	25.578	1.00 21.18	A
ATOM	473	C	PHE		58	44.278	-7.401	28.612	1.00 21.79	A
ATOM	474	ō	PHE		58	44.529	-8.260	27.763	1.00 21.84	A
ATOM	475	И	ALA		59	44.849	-6.202	28.637	1.00 21.80	A
ATOM	476	CA	ALA		59	45.840	-5.801	27.657	1.00 21.67	A
ATOM	477	СВ	ALA		59	46.254	-4.346	27.892	1.00 21.11	A
ATOM	478	C	ALA		59	47.053	-6.711	27.732	1.00 22.06	A
ATOM	479	ō	ALA		59	47.518	-7.213	26.706	1.00 22.53	A
ATOM	480	N	LEU		60	47.561	-6.925	28.945	1.00 19.83	A
ATOM	481	CA	LEU	JA	60	48.729	-7.777	29.116	1.00 20.88	A
MOTA	482	CB	LEC	JA	60	49.163	-7.815	30.585	1.00 20.57	A
ATOM	483	CG	LEU	JA	60	50.060	-6.657	31.053	1.00 24.17	A
MOTA	484	CDI	LEC	JA	60	49.239	-5.392	31.205	1.00 24.16	A
MOTA	485	CD2	LEC	JA	60	50.717	-7.012	32.382	1.00 24.31	A
MOTA	486	C	LEC		60	48.496	-9.193	28.598	1.00 20.44	A
MOTA	487	0	LEU		60	49.367	-9.770	27.955	1.00 21.97	A
ATOM	488	N	THE		61	47.319	-9.749	28.871	1.00 20.69	A
MOTA	489	CA		R A	61		-11.101	28.418	1.00 19.49	A A
MOTA	490	CB		R A	61		-11.629	29.084 30.489	1.00 18.59 1.00 21.12	A
MOTA	491	OG:			61		-11.830 -12.942	28.453	1.00 21.12	A
MOTA	492		2 THE	K A R A	61 61		-11.140	26.903	1.00 19.22	A
MOTA	493	C		K A			-12.059	26.242	1.00 21.19	A
MOTA	494	N		A			-10.142	26.351	1.00 18.05	A
ATOM ATOM	495 496			A Z			-10.092	24.910	1.00 19.26	A
ATOM	497			N A		45.020	-8.910	24.552	1.00 20.51	A
MOTA	498			A N		43.835	-9.324		1.00 22.06	A
ATOM	499		1 AS				-10.482	23.693	1.00 21.71	A
ATOM	500		2 ASI			43.294	-8.371		1.00 20.64	A
ATOM	501			N A		47.270	-9.975		1.00 18.14	A
ATOM	502			N A		47.517	-10.681	23.217	1.00 19.73	A
ATOM	503			E A		48.146				A
MOTA	504	CA	TL	EΑ	63	49.448				A
ATOM	505	CB	IL	E A	63	50.229				A
MOTA	506		2 IL			51.601				A
ATOM	507		1 IL			49.425				A
ATOM	508		1 IL			49.037	-6.092			A
MOTA	509			e a		50.247	-10.212	24.169		A
MOTA	510			E A		51.048	-10.538	23.297		A
ATOM	511			A A		50.028	-10.949	25.247		A
MOTA	512			AA		50.713	-12.222	25.423		A
MOTA	513	CE	AL	A A	64	50.373	-12.816	26.785	1.00 22.29	A

MOTA	514	C	ALA A				-13.158	24.301	1.00 23.03	A
MOTA	515	0	ALA A				-13.939	23.766	1.00 25.08 1.00 23.28	A A
ATOM	516	N CA	VAL A				-13.072 -13.905	23.948 22.888	1.00 23.28	A
ATOM ATOM	517 518	CB	VAL A				-13.840	22.859	1.00 24.28	A
ATOM	519		VAL A				-14.722	21.729	1.00 22.40	A
ATOM	520	CG2	VAL A	6	5		-14.296	24.209	1.00 19.61	A
ATOM	521	C	VAL A				-13.471	21.538	1.00 23.88	A
ATOM	522	0	VAL A				-14.314	20.692	1.00 22.01 1.00 24.00	A A
ATOM	523	N	LEU A				-12.164 -11.692	21.332 20.064	1.00 24.66	A
MOTA MOTA	524 525	CA CB	LEU A				-10.171	20.011	1.00 22.13	A
ATOM	526	CG	LEU A			48.679	-9.228	20.117	1.00 23.81	A
MOTA	527		LEU A		6	49.014	-8.001	19.277	1.00 20.24	· A
ATOM	528		LEU A			47.407	-9.866	19.627	1.00 20.49	A
ATOM	529	C	LEU A				-12.267	19.906	1.00 23.53 1.00 22.08	A A
ATOM	530	0	LEU A				-12.644 -12.303	18.813 21.011	1.00 26.17	A
ATOM ATOM	531 532	N CA	LYS A				-12.832	21.019	1.00 28.99	A
ATOM	533	СВ	LYS A				-12.698	22.421	1.00 29.27	A
ATOM	534	CG	LYS A	A 6	7	55.278	-13.174	22.548	1.00 30.64	A
MOTA	535	CD	LYS A				-13.001	23.976	1.00 32.41	A
· MOTA	536	CE	LYS A				-13.609	24.157 23.199	1.00 35.25 1.00 38.78	A A
MOTA	537	NZ C	LYS A				-13.036 -14.299	20.598	1.00 29.87	A
ATOM ATOM	538 539	0	LYS 2		7		-14.719	19.716	1.00 30.35	A
ATOM	540	N	HIS A		8		-15.066	21.230	1.00 30.48	A
MOTA	541	CA	HIS 2	A 6	8		-16.483	20.922	1.00 31.95	A
MOTA	542	CB	HIS 2		В		-17.097	21.775	1.00 34.42	A A
MOTA	543	CG	HIS 2		8		-18.557 -19.203	21.520 20.826	1.00 38.63 1.00 40.18	A
ATOM	544 545		HIS A		18 . 18		-19.536	21.992	1.00 41.00	A
MOTA MOTA	546		HIS		8		-20.721	21.601	1.00 39.93	A
ATOM	547		HIS .		8		-20.547	20.891	1.00 39.69	A
ATOM	548	C	HIS :	A 6	8		-16.660	19.448	1.00 31.53	A
MOTA	549	0	HIS .		8		-17.447	18.746	1.00 32.07	A n
MOTA	550	N	ASN .		9		-15.928	18.977 17.583	1.00 29.53 1.00 29.99	A A
MOTA	551 552	CA CB	ASN .		59 59		-16.024 -15.173	17.332	1.00 30.27	A
ATOM ATOM	553	CG	ASN .				-15.814	17.885	1.00 31.83	A
ATOM	554		ASN .		9		-16.728	18.703	1.00 32.19	A
MOTA	555	ND2	ASN .	A 6	59		-15.328	17.447	1.00 31.41	A
ATOM	556	C	ASN		59		-15.602	16.638	1.00 30.37	A A
ATOM	557	0	ASN		59		-16.186 -14.593	15.571 17.026	1.00 29.41 1.00 29.86	A
ATOM ATOM	558 559	N CA	LEU		70 70		-14.131	16.175	1.00 31.35	A
ATOM	560	СВ	LEU		70		-12.857	16.751	1.00 28.55	A
MOTA	561	CG	LEU		70	55.190	-12.237	15.950	1.00 28.77	A
MOTA	562	CDI	LEU	A T	70		-11.949	14.519	1.00 28.48	A
MOTA	563		LEU		70		10.957	16.627	1.00 27.89	A A
ATOM	564	C	LEU		70 70		-15.214 -15.422	16.009 14.914	1.00 31.92 1.00 31.72	A
MOTA MOTA	565 566	N O	LEU ASN		71		-15.905	17.097	1.00 34.09	A
ATOM	567	CA	ASN		71		-16.968	17.060	1.00 38.27	A
ATOM	568	CB	asn		71		-17.651	18.427	1.00 39.70	A
ATOM	569	CG	asn		71	56.490	-16.748	19.490	1.00 44.05	A
MOTA	570		LASN		71) -16.955 7 -15.746	20.693 19.049	1.00 44.98 1.00 44.44	A A
MOTA	571 572	C ND:	ASN ASN		71 71		1 -18.003	15.983	1.00 38.32	A
ATOM ATOM	573	ō	ASN		71 71		-18.417		1.00 37.91	· , A
MOTA	574	N	SER		72	54.221	L -18.407	15.919	1.00 39.49	A
ATOM	575	CA	SER	A	72		-19.390		1.00 40.10	A
MOTA	576		SER		72		1 -19.816		1.00 41.05	A A
ATOM	577		SER		72 72		7 -20.763 0 -18.838		1.00 42.44	A
MOTA MOTA	578 579		ser ser		72 72		6 -19.516		1.00 40.90	A
ATOM	580		LEU		72 73		1 -17.608		1.00 39.86	A
ATOM	581				73	53.40	8 -16.973	12.030	1.00 39.32	A
ATOM	582	CB	LEU	A	73		6 -15.632		1.00 38.99	A
ATOM	583				73		1 -15.651			A A
MOTA	584		1 LEU		73		2 -16.860 9 -14.363			A
ATOM ATOM	585 586		TEO 5 TEO		73 73	54.81	6 -16.778	11.492		A
ATOM	587		LEU		73		8 -16.806			A

				_		FF 70A	16 676	12.383	1.00 39.70	A
ATOM	588	N	ILE		74	55.780 -				
ATOM	589	CA	ILE	A	74	57.158 -		11.942	1.00 41.87	A
ATOM	590	CB	ILE	A	74	58.104 -	-16.084	13.123	1.00 41.88	A
ATOM	591	CG2	ILE	A	74	59.552 -	-16.054	12.640	1.00 41.29	A
ATOM	592		ILE		74	57.729	-14.734	13.738	1.00 41.53	A
			ILE		74	58.519		14.990	1.00 40.94	A
MOTA	593					57.599		11.273	1.00 42.04	A
MOTA	594	C	ILE		74					A
ATOM	595	0	ILE	A	74	58.119 •		10.157	1.00 41.12	
ATOM	596	N	LYS	Α	75	57.364 ·	-18.816	11.954	1.00 43.51	A
ATOM	597	CA	LYS	A	75	57.730 ·	-20.125	11.423	1.00 46.61	A
	598	CB	LYS		75	57.470 ·	-21.217	12,466	1.00 47.84	A
ATOM						58.096		13.828	1.00 50.82	A
ATOM	599	CG	LYS		75				1.00 53.97	A
MOTA	600	CD	LYS		75	57.661		14.828		
MOTA	601	CE	LYS	A	75	58.005		16.269	1.00 55.95	· A
MOTA	602	NZ	LYS	A	75	59.472	-21.572	16.531	1.00 56.31	A
ATOM	603	C	LYS		75	56.944	-20.452	10.151	1.00 47.99	A
			LYS		75	57.530		9.106	1.00 48.11	A
MOTA	604	0						10.242	1.00 49.31	A
ATOM	605	N	ARG		76	55.617				
ATOM	606	CA	ARG	A	76	54.763		9.103	1.00 50.89	A
ATOM	607	CB	ARG	A	76	53.287	-20.744	9.530	1.00 53.08	A
ATOM	608	CG	ARG	A	76	52.960	-21.847	10.538	1.00 56.83	A
		CD	ARG		76	51.478		10.574	1.00 58.85	A
ATOM	609					50.620		11.212	1.00 60.24	A
MOTA	610	NE	ARG		76				1.00 61.29	A
ATOM	611	CZ	ARG		76	49.786		10.557		
ATOM	612	NHl	ARG	A	76	49.692	-20.526	9.234	1.00 60.08	A
MOTA	613	NH2	ARG	A	76	49.044	-19.578	11.226	1.00 61.97	A
ATOM	614	С	ARG		76	54.947	-19.871	7.864	1.00 50.93	A
			ARG		76		-20.324	6.747	1.00 51.19	A
ATOM	615	0						8.046	1.00 50.61	A
ATOM	616	N	SER		77		-18.630		1.00 50.08	A
ATOM	617	CA	SER	A	77		-17.745	6.900		
MOTA	618	CB	SER	A	77	55.262	-16.295	7.282	1.00 50.05	A.
ATOM	619	OG	SER	A	77	56.223	-15.787	8.193	1.00 49.23	A
		C	SER		77	57.006	-17.827	6.386	1.00 49.56	A
ATOM	620						-17.015	5.558	1.00 49.40	A
ATOM	621	0	SER		77				1.00 49.24	A
MOTA	622	N	asn	A	78		-18.817	6.866		
MOTA	623	CA.	ASN	Α	78	59.148	-18.982	6.472	1.00 49.14	A
ATOM	624	CB	ASN	A	78	59.256	-19.307	4.976	1.00 48.86	A
ATOM	625	CG	ASN		78	60.668	-19.689	4.558	1.00 48.09	A
			ASN		78		-20.442	5.254	1.00 46.05	A
MOTA	626						-19.182	3.409	1.00 47.78	A
MOTA	627		ASN		78				1.00 49.08	A
MOTA	628	C	ASN	Α	78		-17.667	6.803		
MOTA	629	0	ASN	Α	78		-17.114	6.001	1.00 48.39	A
MOTA	630	N	SER	A	79	59.571	-17.177	8.006	1.00 48.58	A
ATOM	631	CA	SER		79	60.139	-15.945	8.538	1.00 48.38	A
					79		-16.208	9.071	1.00 48.53	A
ATOM	632	CB	SER				-16.612	8.027	1.00 50.05	A
MOTA	633	OG	SER		79					A
ATOM	634	¢	SER	Ł A	79		-14.768	7.573	1.00 47.13	
ATOM	635	0	SER	A S	79	61.197	-14.098	7.444	1.00 47.66	A
ATOM	636	N	THE	A	80	59.069	-14.516	6.887	1.00 45.82	A
ATOM	637	CA	THE		80	59.008	-13.379	5.982	1.00 45.51	A
		CB	THE		80		-13.501	5.016	1.00 47.03	A
MOTA	638						-13.963	5.731	1.00 47.95	A
MOTA	639		l THE		80					A
MOTA	640	CG:	2 THE	ΑS	80		-14.487	3.909	1.00 47.59	
ATOM	641	C	THE	A 5	80		-12.147	6.882	1.00 44.25	A
MOTA	642	0	THE	A S	80	57.835	-11.976	7.556	1.00 43.69	A
ATOM	643		AL		81	59.889	-11.311	6.903	1.00 41.47	A
			ALZ				-10.119	7.740	1.00 38.59	A
MOTA	644							8.039	1.00 38.61	A
ATOM	645		AL			61.363		7.185	1.00 36.89	A
MOTA	646	C	AL			59.168				
MOTA	647	0	ALA	A A	81	58.766		6.018	1.00 35.83	A
MOTA	648	N	AL	A A	82	58.993	-7.920	8.050	1.00 34.86	A
MOTA	649			A A		58.300	-6.690	7.698	1.00 33.41	A
				A A		57.957			1.00 34.17	A
MOTA	650								1.00 32.28	A
MOTA	651			A A		59.141				A
ATOM	652	0	AL	A A	. 82	60.372				
ATOM	653	N	TH	R A	. 83	58.457				A
ATOM	654			R A		59.100	-4.217	4.931		A
ATOM	659			R A		58.377			1.00 34.31	A
	656		1 TH			58.347				A
MOTA										A
ATOM	657		2 TH			59.098				A
MOTA	658	3 C	TH	R A	83	59.041				
MOTA	659	9 0	TH	R A	83	58.029			_	A
MOTA	661	N	AS	N A	84	60.130	-2.062			A
ATOM	66:			N F		60.188		5.858	1.00 34.66	A
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		~	3 037		0.4	C1 C24	-0,252	6.069	1.00 36.13	A
MOTA	662	CB	ASN		84	61.634		7.132	1.00 37.22	A
MOTA	663	CG	asn		84	62.337	-1.045		1.00 37.22	A
MOTA	664		asn		84	61.809	-1.241	8.220		
MOTA	665		asn		84	63.548	-1.497	6.830	1.00 38.89	A
MOTA	666	C	asn		84	59.549	0.267	4.881	1.00 35.51	A
ATOM	667	0	asn	A	84	59.961	0.343	3.724	1.00 38.89	A
MOTA	668	N	GLU	A	85	58.546	1.004	5.344	1.00 34.17	A
ATOM	669	CA	GLU	A	85	57.890	2.001	4.507	1.00 32.82	A
ATOM	670	CB	GLU	A	85	56.427	2.183	4.921	1.00 36.55	A
ATOM	671	CG	GĿŪ	A	85	55.523	0.993	4.645	1.00 42.74	A
MOTA	672	CD	GLU	A	85	55.271	0.782	3.167	1.00 46.65	A
MOTA	673	OE1	GLU	A	85	54.829	1.741	2.494	1.00 49.22	A
ATOM	674	OE2			85	55.508	-0.345	2.679	1.00 48.74	A
ATOM	675	C	GLU		85	58.624	3.328	4.701	1.00 30.10	A
ATOM	676	ō	GLU		85	59.489	3.453	5.571	1.00 27.29	A
ATOM	677	N	VAL		86	58.274	4.308	3.878	1.00 28.67	A
MOTA	678	CA	VAL		86	58.849	5.641	3.951	1.00 27.33	A
ATOM	679	CB	VAL		86	59.146	6.202	2.539	1.00 27.74	A
MOTA	680		VAL		86	59.688	7.637	2.640	1.00 22.06	A
			VAL		86	60.139	5.289	1.815	1.00 25.30	A
MOTA	681		VAL			57.786	6.519	4.614	1.00 27.98	A
ATOM	682	C			86	56.685	6.671	4.086	1.00 28.76	A
ATOM	683	0	VAL		86			5.784	1.00 27.39	A
ATOM	684	N	PRO		87	58.095	7.098		1.00 26.00	A
MOTA	685	CD	PRO		87	59.268	6.861	6.644		
ATOM	686	CA	PRO		87	57.106	7.949	6.458	1.00 28.38	A
MOTA	687	CB	PRO		B7	57.611	7.989	7.899	1.00 26.97	A
MOTA	688	CG	PRO	A	87	59.099	7.915	7.727	1.00 27.97	A
MOTA	689	С	PRO	A	87	56.963	9.341	5.848	1.00 30.15	A
MOTA	690	0	PRO	A	87	57.902	9.871	5.245	1.00 31.62	A
ATOM	691	N	GLU	A	88	55.778	9.922	6.004	1.00 29.70	A
ATOM	692	CA	GLU	A	88	55.489	11.252	5.481	1.00 29.65	A
ATOM	693	CB	GLU	A	88	54.173	11.229	4.699	1.00 32.09	A
ATOM	694	CG	GLU	A	88	54.038	12.330	3.655	1.00 38.40	A
ATOM	695	CD	GLU	A	88	52.790	12.172	2.792	1.00 41.07	A
ATOM	696		GLU		88	51.675	12.411	3.303	1.00 42.35	A
ATOM	697	OE2			88	52.925	11.800	1.604	1.00 43.46	A
ATOM	698	C	GLU		88	55.385	12.191	6.680	1.00 27.98	A
ATOM	699	ō	GLU		88	54.588	11.954	7.597	1.00 26.16	A
	700	N	VAL		89	56.187	13.253	6.672	1.00 23.90	A
ATOM		CA	VAL		89	56.201	14.194	7.788	1.00 21.62	A
ATOM	701				89	57.637	14.358	8.333	1.00 18.36	A
ATOM	702	CB	VAL			57.639	15.295	9.534	1.00 17.11	A
MOTA	703		VAL		89		12.990	8.719	1.00 16.77	A
ATOM	704		VAL		89	58.204		7.483	1.00 21.60	A
MOTA	705	C	VAL		89	55.626	15.575		1.00 21.72	A
MOTA	706	0	VAL		89	55.859	16.143	6.420	1.00 21.72	A
ATOM	707	N	THR		90	54.886	16.115	8.444	1.00 20.62	A
ATOM	708	CA	THR		90	54.269	17.425	8.301		A
ATOM	709	CB	THR		90	52.813	17.303	7.823	1.00 21.90	
ATOM	710	OG1	THR	. A	90	52.770	16.537	6.613	1.00 26.43	A
MOTA	711	CG2	THR	A	90	52.220	18.678	7.558	1.00 23.70	A
MOTA	712	C	THR	A	90	54.264	18.153	9.639	1.00 21.08	A
ATOM	713	0	THR	A	90	53.887	17.578	10.667	1.00 20.41	A
ATOM	714	N	VAL	Α .	91	54.670	19.423	9.618	1.00 19.24	A
MOTA	715	CA	VAI	. A	91	54.712	20.243	10.822	1.00 19.55	A
MOTA	716	СВ	IAV	A	91	56.149	20.739	11.102	1.00 19.97	A
MOTA	717	CG:	L VAI	A	91	56.167	21.629	12.338	1.00 16.82	A
MOTA	718		Z VAI		91	57.072	19.547	11.280	1.00 17.43	A
MOTA	719	C	IAV		91	53.789	21.452	10.703	1.00 19.10	A
ATOM	720	ō	VAI			53.735	22.108	9.666	1.00 20.59	A
ATOM	721	N	PHE			53.059	21.739	11.772	1.00 18.65	A
ATOM	722	CA	PHE			52.146	22.870	11.785	1.00 19.10	A
		CB		A		50.853	22.516	11.030	1.00 18.89	A
ATOM	723					50.176	21,264	11.525	1.00 16.16	A
ATOM	724	CG	PHI				21.331	12.480	1.00 16.77	A
MOTA	725		1 PHI			49.165		11.047	1.00 16.62	A
ATOM	726		2 PHI			50.561			1.00 18.06	A
MOTA	727		1 PHI			48.543	20.168	12.955		A
MOTA	728		2 PHI			49.954		11.511	1.00 18.17	A
ATOM	729			BA		48.936		12.471	1.00 17.05	A
ATOM	730			E A		51.844		13.229	1.00 19.48	
MOTA	731			E A		52.055		14.134	1.00 19.64	A
MOTA	732	N	SE	R A	. 93	51.365		13.445	1.00 18.69	A
MOTA	733	CA	SE	R A	93	51.052		14.792	1.00 19.26	A
MOTA	734	CB	SE	R A	93	51.275		14.921		A
MOTA	735	OG	SE	R A	93	50.435	27.132	14.043	1.00 20.17	A

MOTA	736	C	SER A	A	93	49.618	24.554	15.172	1.00 19.04	A
MOTA	737	0	SER A	A	93	48.748	24.417	14.316	1.00 17.44	A
MOTA	738	N	LYS 2	A	94	49.390	24.418	16.472	1.00 20.26	A
MOTA	739	CA	LYS A	A	94	48.077	24.108	17.010	1.00 21.70	A
MOTA	740	СВ	LYS A		94	48.227	23.670	18.464	1.00 22.45	A
MOTA	741	CG	LYS A		94	46.938	23.273	19.139	1.00 24.42	A
ATOM	742	CD	LYS A		94	47.189	22.867	20.587	1.00 25.48	A
ATOM	743	CE	LYS A		94	45.881	22.548	21.297	1.00 25.73	A
MOTA	744	NZ	LYS A		94	45.122	21.533 25.340	20.517 16.921	1.00 26.34	A A
ATOM	745	C	LYS A		94 94	47.169 45.984	25.235	16.598	1.00 20.95	A
ATOM ATOM	746 747	N O	SER I		95	47.742	26.505	17.212	1.00 24.82	A
ATOM	748	CA	SER 2		95	47.013	27.769	17.172	1.00 27.69	A
ATOM	749	CB	SER A		95	46.969	28.408	18.565	1.00 26.33	A
ATOM	750	OG	SER A		95	46.202	27.635	19.468	1.00 32.56	A
ATOM	751	C	SER I		95	47.688	28.747	16.219	1.00 27.36	A
ATOM	752	0	SER A	A	95	48.824	28.529	15.797	1.00 27.94	A
ATOM	753	N	PRO 2	A	96	46.985	29.830	15.849	1.00 27.27	A
ATOM	754	CD	PRO 1	A	96	45.611	30.232	16.193	1.00 28.85	A
MOTA	755	CA	PRO I	A	96	47.606	30.801	14.946	1.00 26.90	A
MOTA	756	CB	PRO 2		96	46.471	31.788	14.663	1.00 28.13	A
ATOM	757	CG	PRO 2		96	45.634	31.719	15.907	1.00 28.36	A
ATOM	758	C	PRO 2		96	48.786	31.421	15.700	1.00 24.92 1.00 24.65	A A
ATOM	759	0	PRO		96	48.757 49.828	31.556 31.786	16.925 14.973	1.00 24.03	A
ATOM	760	N CA	VAL Z		97 97	51.016	32.332	15.601	1.00 25.15	A
MOTA MOTA	761 762	CB	VAL :		97	52.261	32.087	14.715	1.00 26.78	A
ATOM	763		VAL		97	53.531	32.372	15.508	1.00 26.15	A
ATOM	764		VAL.		97	52.255	30.659	14.198	1.00 26.15	A
ATOM	765	C	VAL .		97	50.935	33.820	15.920	1.00 25.62	A
MOTA	766	0	VAL .	A	97	50.624	34.638	15.054	1.00 25.01	A
ATOM	767	N	THR .	A	98	51.207	34.157	17.175	1.00 24.46	A
MOTA	768	CA	THR .	A	98	51.212	35.542	17.627	1.00 25.36	A
ATOM	769	CB	THR .		98	49.835	35.941	18.283	1.00 25.29	A
MOTA	770		THR .		98	50.030	37.008	19.217	1.00 30.50	A
MOTA	771		THR .		98	49.196	34.771	18.985	1.00 29.80	A
ATOM	772	С	THR		98	52.382	35.678	18.605	1.00 24.87	A A
ATOM	773	0	THR		98	52.499	34.902	19.554 18.344	1.00 23.01 1.00 25.94	A A
ATOM	774	N	LEU		99	53.273 54.445	36.634 36.843	19.198	1.00 28.02	A
ATOM ATOM	775 776	CA CB	LEU		99 99	55.194	38.114	18.797	1.00 31.12	A
ATOM	777	CG	LEU		99	55.950	38.211	17.469	1.00 35.44	A
ATOM	778		LEU		99	56.650	39.577	17.416	1.00 35.45	A
ATOM	779		LEU		99	56.970	37.087	17.341	1.00 35.62	A
ATOM	780	C	LEU		99	54.135	36.932	20.689	1.00 27.10	A
MOTA	781	0	LEU	A	99	53.201	37.616	21.097	1.00 25.34	A
MOTA	782	N	GLY			54.935	36.233	21.492	1.00 26.71	A
MOTA	783	CA	GLY			54.762	36.253	22.935	1.00 26.48	A
ATOM	784	C	GLY			53.635	35.398	23.479	1.00 26.32	A
MOTA	785	0	GLY			53.428	35.323	24.695	1.00 25.37 1.00 25.16	A A
ATOM	786	N	GLN			52.913 51.796	34.734 33.896	22.585 22.999	1.00 25.74	A
MOTA MOTA	787 788	CA CB	GLN GLN			50.573	34.219	22.143	1.00 28.06	A
ATOM	789	CG	GLN			49.258	33.911	22.814	1.00 30.50	A
ATOM	790	CD	GLN			49.123	34.599	24.162	1.00 32.88	A
ATOM	791		GLN			48.953	35.820	24.251	1.00 30.83	A
ATOM	792	NE2	GLN	A	101	49.202	33.813	25.221	1.00 33.04	A
MOTA	793	C	GLN			52.117	32.409	22.901	1.00 24.01	A
MOTA	794	0	GLN			52.280	31.881	21.807	1.00 24.25	A
MOTA	795	N	PRO			52.199	31.715	24.051	1.00 22.08	A A
MOTA	796	CD	PRO			51.959	32.244	25.410	1.00 22.41 1.00 21.37	A
ATOM	797	CA			102	52.500	30.278	24.096 25.526	1.00 21.61	Ā
MOTA	798	CB			102	52.136 52.521	29.898 31.147	26.297	1.00 21.90	A
MOTA MOTA	799 800	CG			102 102	51.706	29.480	23.068	1.00 21.30	A
ATOM	801	0			102	50.496	29.644	22.947	1.00 21.93	A
ATOM	802	N			103	52.396	28.618	22.327	1.00 18.86	A
ATOM	803	CA			103	51.749	27.802	21.305	1.00 17.69	A
ATOM	804	CB			103	52.040	28.379	19.913	1.00 17.99	A
ATOM	805	ÇG	asn	A	103	50.899	28.162	18.929	1.00 18.28	A
MOTA	806		l asn			50.348	27.060	18.808	1.00 17.82	A
ATOM	807		2 ASN			50.549	29.223	18.204	1.00 17.71	A A
ATOM	808	C			103	52.281		21.385	1.00 15.57 1.00 14.67	A
MOTA	809	0	ASN	A	103	53.000	26.012	22.310	T.00 T4.01	•1

ATOM	810	N	ILE A	104	51.918	25.565	20.397	1.00 15.80	A
ATOM	811	CA	ILE A	104	52.335	24.177	20.328	1.00 13.66	A
MOTA	812	CB	ILE A	104	51.255	23.235	20.888	1.00 15.40	A
MOTA	813		ILE A		51.589	21.792	20.539	1.00 13.82	A
ATOM	814		ILE A		51.132	23.421	22.400	1.00 17.40	A
ATOM	815		ILE A		50.129	22.494	23.047 18.896	1.00 18.65 1.00 14.36	A A
ATOM	816	C	ILE A		52.588 51.716	23.775 23.924	18.052	1.00 16.86	A
ATOM ATOM	817 818	o N	TEG Y		53.785	23.272	18.616	1.00 15.67	A
ATOM	819	CA	LEU A		54.090	22.822	17.272	1.00 15.52	A
ATOM	820	СВ	LEU A		55.568	22.978	16.940	1.00 15.73	A
ATOM	821	CG	LEU A		56.058	24.391	16.649	1.00 20.75	A
ATOM	822		LEU A		57.400	24.298	15.919	1.00 20.19	A
ATOM	823	CD2	LEU A	105	55.030	25.141	15.791	1.00 21.31	A
MOTA	824	C	LEU A		53.709	21.362	17.202	1.00 15.97	A
MOTA	825	0	LEU A		53.968	20.589	18.133	1.00 14.11	A
ATOM	826	N	ILE A		53.078	20.993	16.099	1.00 14.18 1.00 15.40	A A
MOTA	827	CA CB	ILE A		52.643 51.122	19.630 19.576	15.903 15.636	1.00 15.11	A
ATOM ATOM	828 829		ILE A		50.661	18.135	15.592	1.00 12.46	A
ATOM	830		ILE A		50.380	20.354	16.734	1.00 15.51	A
ATOM	831		ILE A		48.862	20.413	16.565	1.00 12.83	A
ATOM	832	C	ILE A		53.381	19.011	14.725	1.00 16.48	A
ATOM	833	0	ILE A	106	53.484	19.607	13.651	1.00 17.37	A
ATOM	834	N	CYS A	107	53.900	17.811	14.944	1.00 17.86	A
ATOM	835	CA	CYS A	107	54.621	17.083	13.917	1.00 18.32	A
ATOM	836	C	CYS A		53.886	15.776	13.663	1.00 18.29	A
ATOM	837	0	CYS A		53.846	14.909	14.533	1.00 18.13	A A
ATOM	838	CB	CYS A		56.041	16.792	14.382 13.158	1.00 19.33 1.00 25.82	A
MOTA MOTA	839	SG	CYS A		57.029 53.304	15.889 15.649	12.472	1.00 23.82	Ā
ATOM	840 841	N CA	TEO Y		52.556	14.456	12.088	1.00 18.82	A
ATOM	842	CB.	LEU A		51.330	14.850	11.252	1.00 20.17	A
ATOM	843	CG	LEU A		50.129	13.900	11.053	1.00 21.48	A
MOTA	844		LEU A	108	49.623	14.049	9.624	1.00 20.62	A
ATOM	845	CD2	LEU A	108	50.493	12.458	11.316	1.00 18.40	A
MOTA	846	C	LEU A		.53.445	13.538	11.252	1.00 19.49	A
MOTA	847	0	LEU A	•	53.841	13.892	10.144	1.00 20.39	A
MOTA	848	N	VAL A		53.760	12.368	11.789	1.00 18.45	A
MOTA	849	CA	VAL A		54.586	11.398	11.087	1.00 19.04 1.00 18.71	A A
MOTA	850	CB	VAL F		55.665 56.626	10.805 9.923	12.042 11.279	1.00 15.16	A
ATOM ATOM	851 852		VAL A		56.431	11.949	12.729	1.00 17.68	A
ATOM	853	C	VAL 2	•	53.611	10.322	10.606	1.00 20.50	A
ATOM	854	ō	VAL 2		53.115	9.516	11.393	1.00 21.55	A
MOTA	855	N	ASP A		53.326	10.337	9.308	1.00 21.50	A
ATOM	856	CA	ASP A	110	52.376	9.407	8.700	1.00 21.95	A
ATOM	857	CB	ASP A	110	51.493	10.165	7.701	1.00 22.25	A
MOTA	858	CG	ASP A		50.084	9.612	7.622	1.00 24.20	A
MOTA	859		ASP A		49.874	8.435	7.989	1.00 23.87	A
MOTA	860		ASP A		49.182	10.356	7.182	1.00 25.94 1.00 21.53	A A
ATOM	861	C	ASP A		53.059 54.273	8.240 8.254	7.985 7.782	1.00 18.80	A
ATOM	862 863	N	ASP A	A 111	52.254	7.245	7.603	1.00 23.78	A
ATOM ATOM	864	CA		A 111	52.706	6.037	6.900	1.00 23.32	A
ATOM	865	СВ		A 111	53.046	6.360	5.437	1.00 24.67	A
ATOM	866	CG		A 111	53.181	5.102	4.575	1.00 31.76	A
ATOM	867		ASN I		52.291	4.240	4.567	1.00 31.05	A
MOTA	868	ND2	ASN 3	A 111	54.292	4.994	3.842	1.00 29.09	A
ATOM	869	C		A 111	53.905	5.389	7.587	1.00 23.68	A
MOTA	870	0		A 111	54.953	5.156	6.976	1.00 22.88	A
MOTA	871	N		A 112	53.738	5.090	8.868	1.00 22.97 1.00 20.73	A A
MOTA	872	CA		A 112	54.797	4.473	9.646 11.108	1.00 20.13	A
ATOM ATOM	873	CB	ILE :	A 112	54.791 55.979	4.967 4.363	11.864	1.00 15.53	A
ATOM	874 875		ILE.		54.833	6.495	11.158	1.00 19.14	A
MOTA	876		LILE		54.671	7.058	12.575	1.00 20.42	A
MOTA	877	C C		A 112	54.658	2.960	9.699	1.00 22.54	A
ATOM	878	ō		A 112	53.605	2.436	10.054	1.00 22.65	A
MOTA	879	N		A 113	55.732	2.266	9.343	1.00 21.37	A
MOTA	880	CA		A 113	55.769	0.819	9.412	1.00 21.74	A
MOTA	881	CB		A 113	54.742	0.167	8.483	1.00 21.64 1.00 21.22	A A
MOTA	882	CG		A 113	54.451		8.850 9.856	1.00 20.25	A
MOTA	883	CD:	L PHE	W TT2	53.528	-1.543	٥.٥٥٥		-•

ATOM	884	CD2	PHE A 113	55.183	-2.296	8.285	1.00 20.76	A
MOTA	885	CEl	PHE A 113	53.341	-2.848	10.302	1.00 19.85	A
ATOM	886		PHE A 113	55.008	-3.607	8.721	1.00 20.75	A
MOTA	887	CZ	PHE A 113	54.086	-3.887	9.735	1.00 21.24	A
ATOM	888	C	PHE A 113	57.157	0.329	9.042	1.00 21.21	A A
MOTA MOTA	889 890	O N	PHE A 113 PRO A 114	57.700 57.765	0.719 -0.509	8.011 9.893	1.00 19.97 1.00 22.22	A
ATOM	891	CD	PRO A 114	59.118	-1.018	9.614	1.00 22.88	A.
ATOM	892	CA	PRO A 114	57.263	-1.040	11.170	1.00 23.38	A
ATOM	893	СВ	PRO A 114	58.340	-2.045	11.571	1.00 23.68	A
ATOM	894	CG	PRO A 114	59.592	-1.435	10.984	1.00 23.26	A
MOTA	895	C	PRO A 114	57.078	0.059	12.221	1.00 24.33	A
ATOM	896	0	PRO A 114	57.571	1.174	12.054	1.00 24.35	A
ATOM	897	И	PRO A 115 PRO A 115	56.363 55.579	-0.247 -1.472	13.319 13.567	1.00 24.59 1.00 22.60	A A
ATOM ATOM	898 899	CD CA	PRO A 115	56.135	0.751	14.372	1.00 23.79	A
ATOM	900	CB	PRO A 115	54.923	0.194	15.107	1.00 23.96	A
MOTA	901	CG	PRO A 115	55.129	-1.291	14.998	1.00 23.45	A
ATOM	902	C	PRO A 115	57.33 7	0.996	15.289	1.00 24.97	A
ATOM	903	0	PRO A 115	57.322	0.670	16.482	1.00 23.11	A
ATOM	904	N	VAL A 116	58.380	1.573	14.705	1.00 24.77	A
MOTA	905	CA	VAL A 116	59.607	1.902	15.423 15.135	1.00 24.05 1.00 26.45	A A
ATOM	906	CB	VAL A 116 VAL A 116	60.733 61.977	0.881 1.250	15.133	1.00 24.89	A
ATOM ATOM	907 908		VAL A 116	60.267	-0.539	15.470	1.00 26.43	A
ATOM	909	C	VAL A 116	60.043	3.254	14.875	1.00 24.47	A
ATOM	910	ō	VAL A 116	60.340	3.381	13.684	1.00 23.94	A
MOTA	911	N	VAL A 117	60.088	4.269	15.728	1.00 22.43	A
ATOM	912	CA	VAL A 117	60.472	5.577	15.239	1.00 22.18	A
ATOM	913	CB	VAL A 117	59.247	6.277	14.565	1.00 21.24	A
ATOM	914		VAL A 117	58.276	6.807 7.387	15.631 13.653	1.00 17.87 1.00 19.98	A A
MOTA	915 916	CG2	VAL A 117 VAL A 117	59.710 61.035	6.484	16.326	1.00 23.40	A
ATOM ATOM	917		VAL A 117	60.743	6.323	17.512	1.00 22.77	A
ATOM	918	N	ASN A 118	61.868	7.427	15.909	1.00 24.87	A
ATOM	919	CA	ASN A 118	62.434	8.398	16.833	1.00 25.96	A
MOTA	920	CB	ASN A 118	63.970	8.341	16.858	1.00 29.36	A
MOTA	921	CG	ASN A 118	64.506	7.213	17.728	1.00 31.24	A
MOTA	922		ASN A 118	63.885	6.833	18.722	1.00 34.20	A A
MOTA	923		ASN A 118 ASN A 118	65.679 61.989	6.694 9.746	17.374 16.312	1.00 34.04 1.00 24.87	A
MOTA MOTA	924 925	С О	ASN A 118	62.298	10.112	15.177	1.00 26.17	A
ATOM	926	N	ILE A 119	61.229	10.468	17.122	1.00 23.82	A
MOTA	927	CA	ILE A 119	60.774	11.793	16.727	1.00 23.07	A
MOTA	928	CB	ILE A 119	59.231	11.892	16.711	1.00 22.65	A
MOTA	929		ILE A 119	58.797	13.197	16.051	1.00 18.01	A
MOTA	930		ILE A 119	58.642	10.716	15.936	1.00 21.02 1.00 21.88	A A
MOTA	931	CDI	ILE A 119 ILE A 119	57.135 61.323	10.714 12.771	15.921 17.754	1.00 22.76	A
MOTA MOTA	932 933	Ö	ILE A 119	61.013	12.680	18.940	1.00 22.92	A
ATOM	934	N	THR A 120	62.162	13.691	17.303	1.00 23.11	A
ATOM	935	CA	THR A 120	62.737	14.673	18.205	1.00 23.65	A
ATOM	936	CB	THR A 120	64.216	14.363	18.495	1.00 25.23	A
MOTA	937		THR A 120	64.921	14.199	17.258	1.00 26.55	A
MOTA	938		THR A 120	64.335 62.622	13.081 16.064	19.331 17.616	1.00 23.93 1.00 23.20	A A
ATOM	939 940	C O	THR A 120 THR A 120	62.437	16.232	16.412	1.00 23.15	A
ATOM ATOM	941	N	TRP A 121	62.725	17.069	18.470	1.00 22.54	A
MOTA	942	CA	TRP A 121		18.432	17.998	1.00 21.37	A
MOTA	943	CB	TRP A 121	61.563	19.196	18.791	1.00 19.43	. А
MOTA	944	CG	TRP A 121		18.679	18.616	1.00 18.76	A
ATOM	945		TRP A 121		19.179	17.703	1.00 19.96	A
ATOM	946		TRP A 121		18.454	17.931 16.715	1.00 18.06 1.00 16.07	A A
ATOM	947 948		TRP A 121		20.178 17.694	19.330	1.00 18.18	A
ATOM ATOM	948		TRP A 121		17.553	18.929	1.00 19.21	A
ATOM	950		TRP A 121		18.694	17.210	1.00 16.20	A
ATOM	951		TRP A 121		20.419	16.000	1.00 16.43	A
MOTA	952		TRP A 121		19.679	16.252	1.00 17.37	A
MOTA	953	C	TRP A 121		19.178	18.097	1.00 22.88	A N
MOTA	954	0	TRP A 121		18.937	18.992 17.164	1.00 22.75 1.00 23.24	A A
ATOM ATOM	955 956	N CA	LEU A 122 LEU A 122		20.100 20.930	17.136	1.00 22.66	A
ATOM	957	CB	LEU A 122		20.699	15.850	1.00 23.05	A

N THOM	050	CG	LEU 2	. 1-	22	66.638	19.293	15.563	1.00	22 23	A
ATOM ATOM	958 959		LEU 1			67.404	19.326	14.253	1.00		A
MOTA	960		LEU /			67.542	18.830	16.700		20.21	A
ATOM	961		LEU A			64.837	22.376	17,186		23.52	A
ATOM	962		LEU 1			63.830	22.752	16.572		21.74	A
ATOM	963		SER A			65.579	23.174	17.945		23.69	A
ATOM	964	CA	SER 2			65.330	24.597	18.063		24.10	A
ATOM	965	СВ	SER I			64.998	24.983	19.504		25.22	A
ATOM	966	OG	SER 2			64.735	26.373	19.591	1.00	25.55	A
ATOM	967	¢	SER			66.664	25,200	17.650	1.00	24.79	A
ATOM	968	ō	SER .			67.670	25.014	18.335	1.00	23.07	A
ATOM	969	N	ASN :			66.666	25.903	16.521	1.00	25.02	A
ATOM	970	CA	ASN .			67.880	26.513	15.986	1.00	25.63	A
ATOM	971	CB	ASN .	A 1:	24	68.351	27.676	16.868	1.00	24.46	A
MOTA	972	CG	ASN .	A 1:	24	67.376	28.839	16.873	1.00	25.33	A
MOTA	973	OD1	ASN .	A 1:	24	66.636	29.056	15.907	1.00	26.04	A
MOTA	974	ND2	ASN .	A 1	24	67.381	29.606	17.956		21.77	A
MOTA	975	С	ASN .	A 1	24	69.006	25.487	15.838		26.53	A
MOTA	976	0	ASN .			70.132	25.706	16.301		26.36	A
MOTA	977	N	GLY			68.684	24.361	15.205		24.78	A
ATOM	978	CA	GLY			69.669	23.326	14.964		26.09	A
MOTA	979	С	GLY			70.030	22.377	16.089		27.35	A A
ATOM	980	0	GLY			70.728	21.395	15.846		28.21	A
MOTA	981	N	HIS			69.566	22.645	17.307		28.65 30.12	A
ATOM	982	CA	HIS			69.889	21.774	18.430 19.408		32.68	A
ATOM	983	CB	HIS			70.816	22.507	19.996		35.25	A
ATOM	984	CG	HIS			70.226	23.750 25.044	19.601		36.90	A
ATOM	985		HIS			70.296 69.475	23.743	21.151		35.93	A
MOTA	986		HIS			69.110	24.979	21.445		36.88	A
ATOM	987		HIS			69.595	25.788	20.520		36.73	A
ATOM	988 989	C	HIS			68.661	21.220	19.149		30.87	A
MOTA MOTA	990	o	HIS			67.634	21.889	19.270		31.49	A
MOTA	991	N	SER			68.789	19.990	19.635		30.93	A
ATOM	992	CA	SER			67.697	19.286	20.302	1.00	33.08	A
MOTA	993	СВ	SER			68.165	17.889	20.714	1.00	33.91	A
ATOM	994	OG	SER			69.231	17.979	21.645	1.00	38.34	A
ATOM	995	C	SER			67.050	19.971	21.501	1.00	32.98	A
ATOM	996	0	SER	A 1	.27	67.708	20.654	22.288	1.00	34.83	A
ATOM	997	N	VAL	A 1	.28	65.743	19.770	21.624	1.00	32.42	A
MOTA	998	CA	VAL	A 1	.28	64.960	20.325	22.716	1.00	31.29	A
ATOM	999	CB	VAL	A 1	.28	63.645	20.921	22.202		30.48	A
MOTA	1000	CG1	VAL	A 1	.28	62.856	21.520	23.358		27.06	A
MOTA	1001	CG2	VAL	A 1	.28	63.937	21.970	21.142		28.52	A
ATOM	1002	C	VAL			64.645	19.183	23.669		32.28	A
MOTA	1003	0	VAL			64.275	18.093	23.237		32.80	A
MOTA	1004	N	THR			64.786	19.437	24.965 25.981		33.30 33.70	A A
MOTA	1005	CA	THR			64.546	18.411 18.344			34.52	A
ATOM	1006	СВ	THR			65.740	19.643	26.966 27.528		38.18	A
ATOM	1007		THR			65.969 67.006	17.898	26.245		34.60	A
MOTA	1008	C	THR			63.257	18.591	26.791		32.08	A
ATOM MOTA	1009 1010	0	THR			62.645	17.615	27.220		34.04	A
ATOM	1011	N	GLU			62.843	19.835	26.993	1.00	28.85	A
ATOM	1012	CA	GLU			61.639	20.119	27.762	1.00	26.09	A
MOTA	1013	СВ	GLU			61.926	21.236	28.770	1.00	28.58	A
MOTA	1014	CG	GLU	A :	130	62.962	20.894	29.822	1.00	32.87	A
ATOM	1015	CD	GLU			62.592	19.654	30.609	1.00	35.34	A
ATOM	1016		GLU	A :	130	61.392	19.475	30.907	1.00	37.85	A
ATOM	1017	OE2	GLU	A :	130	63.501	18.865	30.941	1.00	36.29	A
ATOM	1018	C	GLU	A :	130	60.451	20.534	26.893		23.53	A
ATOM	1019	0	GLU	A:	130	60.629	21.166	25.859		19.76	A
MOTA	1020	N	GLY			59.243		27.334		21.13	A
MOTA	1021	CA	GLY			58.046		26.601		20.14	A
MOTA	1022	C	GLY			57.693		25.421		20.64	A
MOTA	1023	0	GLY			56.989		24.507		20.11	A
MOTA	1024	N	VAL			58.164				18.28	A
MOTA	1025	CA.	VAL			57.899		24.355		20.08	A
ATOM	1026	CB	VAL			59.230		23.767		20.35	A A
MOTA	1027		VAL			58.946		22.772		22.11	A A
ATOM	1028		VAL			60.006				20.17	A
MOTA	1029	C		A		57.027				18.65	A
MOTA	1030	0			132 133	57.194 56.094				17.90	A
ATOM	1031	И	DEK	. A		50.034	45.540				

ATOM	1032	CA	SER A 133	55.238	14.802	24.215	1.00 18.16	A
MOTA	1033	CB	SER A 133	54.045	15.206	25.094	1.00 18.24	A
MOTA	1034	OG	SER A 133	53.202	16.143	24.440	1.00 24.24	A
ATOM	1035	C	SER A 133	54.738	14.200	22.914	1.00 16.52	A A
MOTA	1036	0	SER A 133 GLU A 134	54.876 54.166	14.794 13.009	21.843 22.996	1.00 16.18 1.00 17.45	A
ATOM ATOM	1037 1038	n Ca	GLU A 134	53.653	12.369	21.800	1.00 18.50	A
ATOM	1039	CB	GLU A 134	54.797	11.661	21.050	1.00 22.31	A
ATOM	1040	CG	GLU A 134	55.475	10.513	21.801	1.00 24.62	A
MOTA	1041	CD	GLU A 134	56.610	9.859	20.992	1.00 28.65	A
MOTA	1042		GLU A 134	56.932	8.680	21.254	1.00 29.58	A
ATOM	1043		GLU A 134	57.188	10.521	20.099	1.00 27.96	A
MOTA	1044	C	GLU A 134	52.523	11.389 11.003	22.087 23.234	1.00 18.44 1.00 17.30	A A
ATOM ATOM	1045 1046	Ŋ	GLU A 134 THR A 135	52.279 51.824	11.003	21.027	1.00 16.71	A
ATOM	1047	CA	THR A 135	50.733	10.059	21.119	1.00 15.49	A
ATOM	1048	CB	THR A 135	49.738	10.246	19.967	1.00 16.16	A
ATOM	1049	OG1	THR A 135	50.369	9.867	18.731	1.00 16.02	A
ATOM	1050	CG2	THR A 135	49.280	11.697	19.879	1.00 14.19	A
MOTA	1051	С	THR A 135	51.346	8.682	20.946	1.00 17.19 1.00 17.26	A A
MOTA	1052	0	THR A 135	52.551 50.519	8.554 7.650	20.733 21.047	1.00 17.20	A
ATOM ATOM	1053 1054	n ca	SER A 136 SER A 136	51.001	6.297	20.818	1.00 15.92	A
ATOM	1055	СВ	SER A 136	50.035	5.266	21.416	1.00 16.85	A
MOTA	1056	OG	SER A 136	49.756	5.532	22.781	1.00 18.22	A
MOTA	1057	C	SER A 136	50.967	6.187	19.294		A
MOTA	1058	0	SER A 136	50.715	7.169	18.596	1.00 17.25	A
MOTA	1059	N	PHE A 137	51.236	5.003	18.767	1.00 17.08 1.00 15.67	A A
ATOM	1060	CA	PHE A 137 PHE A 137	51.155 51.874	4.806 3.519	17.333 16.936	1.00 13.47	A
MOTA MOTA	1061 1062	CB	PHE A 137	53.363	3.628	16.951	1.00 14.48	A
ATOM	1063		PHE A 137	54.037	4.255	15.907	1.00 15.82	A
ATOM	1064		PHE A 137	54.100	3.112	18.010	1.00 15.21	A
ATOM	1065	CEI	PHE A 137	55.427	4.367	15.918	1.00 15.72	A
ATOM	1066		PHE A 137	55.490	3.220	18.031	1.00 15.14	A
ATOM	1067	cz	PHE A 137	56.152	3.848	16.983 17.067	1.00 14.35 1.00 16.21	A A
MOTA	1068	C 0	PHE A 137 PHE A 137	49.659 49.037	4.657 3.767	17.622	1.00 18.05	A
ATOM ATOM	1069 1070	И	LEU A 138	49.074	5.534	16.259	1.00 17.51	A
ATOM	1071	CA	LEU A 138	47.648	5.433	15.953	1.00 19.20	A
ATOM	1072	CB	LEU A 138	47.017	6.822	15.800	1.00 20.80	A
MOTA	1073	CG	LEU A 138	46.809	7.688	17.044	1.00 23.47	A
MOTA	1074		LEU A 138	46.141	6.879	18.144 17.529	1.00 24.75 1.00 27.62	A A
MOTA	1075	CD2	LEU A 138	48.140 47.490	8.212 4.637	14.658	1.00 18.41	A
MOTA MOTA	1076 1077	0	LEU A 138	48.218	4.862	13.698	1.00 16.16	A
ATOM	1078	N	SER A 139	46.530	3.716	14.630	1.00 18.51	A
MOTA	1079	CA	SER A 139	46.333	2.863	13.460	1.00 17.61	A
MOTA	1080	CB	SER A 139	45.481	1.656	13.836	1.00 18.17	A
MOTA	1081	OG	SER A 139	44.134	2.036	14.040 12.216	1.00 20.80 1.00 17.44	A A
MOTA	1082	C 0	SER A 139 SER A 139	45.729 45.122	3.510 4.578	12.216	1.00 17.44	A
MOTA MOTA	1083 1084	И	LYS A 140	45.908	2.822	11.088	1.00 18.56	A
ATOM	1085	CA	LYS A 140	45.402	3.237	9.778	1.00 18.37	A
ATOM	1086	CB	LYS A 140	46.543	3.751	8.895	1.00 21.60	A
ATOM	1087	CG	LYS A 140	47.149	5.085	9.326	1.00 24.86	A
MOTA	1088	CD	LYS A 140	46.513	6.267	8.602	1.00 30.27 1.00 29.93	A A
MOTA	1089	CE	LYS A 140 LYS A 140	46.961 48.440	6.345 6.349	7.150 7.038	1.00 29.93	A
ATOM ATOM	1090 1091	NZ C	LYS A 140	44.773	2.012	9.118	1.00 17.79	A
ATOM	1092	ŏ	LYS A 140	45.106	0.878	9.458	1.00 17.76	A
ATOM	1093	N	SER A 141	43.882	2.234	8.160	1.00 18.54	A
ATOM	1094	CA	SER A 141	43.220	1.124	7.481	1.00 21.55	A
MOTA	1095	CB	SER A 141	42.047	1.634	6.630	1.00 21.05 1.00 28.41	A A
ATOM	1096	OG	SER A 141 SER A 141	42.490 44.154	2.482 0.263	5.588 6.625	1.00 28.41	A
ATOM	1097 1098	C	SER A 141 SER A 141	44.154	-0.885	6.332	1.00 21.42	A
MOTA MOTA	1099	N	ASP A 142	45.311		6.226		A
ATOM	1100	CA	ASP A 142	46.234				A
MOTA	1101	CB	ASP A 142	47.008				A
MOTA	1102	CG		47.949				A A
ATOM	1103		1 ASP A 142 2 ASP A 142	47.837 48.799				A
MOTA MOTA	1104 1105	C C	ASP A 142	47.176				A
222 Ora		-						

MOTA	1106	0	ASP A 142	48.127	-1.416	5.946	1.00 19.21	A
MOTA	1107	N	HIS A 143	46.885	-0.626	7.659	1.00 18.99	A A
ATOM	1108	CA	HIS A 143	47.637 47.686	-1.295 -2.792	8.706 8.409	1.00 17.27 1.00 16.45	A
MOTA MOTA	1109 1110	CB CG	HIS A 143	46.329	-3.396	8.190	1.00 18.33	A
ATOM	1111		HIS A 143	45.860	-4.211	7.213	1.00 17.59	A
ATOM	1112		HIS A 143	45.262	-3.151	9.032	1.00 15.97	A
ATOM	1113	CE1	HIS A 143	44.194	-3.786	8.580	1.00 19.46	A
MOTA	1114		HIS A 143	44.529	-4.436	7.478	1.00 18.06	A A
ATOM	1115	C	HIS A 143	49.019	-0.749 -1.401	9.030 9.715	1.00 19.46 1.00 19.95	A
ATOM ATOM	1116 1117	O N	HIS A 143 SER A 144	49.812 49.301	0.454	8.536	1.00 19.70	A
ATOM	1118	CA	SER A 144	50.542	1.141	8.852	1.00 20.18	A
ATOM	1119	CB	SER A 144	51.018	2.011	7.678	1.00 19.91	A
MOTA	1120	OG	SER A 144	50.099	3.044	7.364	1.00 23.64	A
MOTA	1121	C	SER A 144	50.109	2.018	10.034	1.00 19.40 1.00 19.70	A A
ATOM	1122	0	SER A 144	48.970 50.986	1.906 2.883	10.499 10.525	1.00 16.99	A
MOTA MOTA	1123 1124	N CA	PHE A 145 PHE A 145	50.614	3.728	11.649	1.00 16.06	A
ATOM	1125	CB	PHE A 145	51.325	3.274	12.929	1.00 16.25	A
ATOM	1126	CG	PHE A 145	51.062	1.841	13.297	1.00 19.53	A
ATOM	1127	CD1	PHE A 145	51.754	0.807	12.672	1.00 20.17	A
MOTA	1128		PHE A 145	50.114	1.522	14.263	1.00 18.18	A
MOTA	1129		PHE A 145	51.505 49.856	-0.525 0.193	13.005 14.606	1.00 21.33 1.00 19.50	A A
MOTA	1130		PHE A 145	50.553	-0.831		1.00 20.23	A
ATOM ATOM	1131 1132	CZ C	PHE A 145	50.955	5.182	11.419	1.00 15.69	A
ATOM	1133	ŏ	PHE A 145	51.548	5.538	10.404	1.00 16.69	A
ATOM	1134	N	PHE A 146	50.530	6.021	12.357	1.00 14.53	A
MOTA	1135	CA	PHE A 146	50.869	7.429	12.332	1.00 16.67 1.00 16.59	A A
MOTA	1136	CB	PHE A 146	49.841	8.279 8.528	11.552 12.259	1.00 15.25	A
ATOM	1137	CG	PHE A 146 PHE A 146	48.535 48.370	9.644	13.071	1.00 15.42	A
MOTA MOTA	1138 1139		PHE A 146	47.433	7.708	12.019	1.00 16.06	A
MOTA	1140		PHE A 146	47.123	9.952	13.629	1.00 17.50	A
ATOM	1141	CE2	PHE A 146	46.180	8.003	12.571	1.00 16.80	A
MOTA	1142	CZ	PHE A 146	46.023	9.126	13.375	1.00 17.47 1.00 17.00	A A
MOTA	1143	C	PHE A 146	51.017 50.345	7.841 7.308	13.783 14.661	1.00 17.00	A
MOTA	1144 1145	O N	PHE A 146 LYS A 147	51.950	8.747	14.032	1.00 17.82	A
ATOM ATOM	1145	CA	LYS A 147	52.224	9.221	15.377	1.00 18.67	A
MOTA	1147	CB	LYS A 147	53.540	8.604	15.863	1.00 20.48	A
MOTA	1148	CG	LYS A 147	53.771	8.668	17.359	1.00 25.54	A
MOTA	1149	CD	LYS A 147	54.822	7.645	17.774	1.00 29.96 1.00 30.05	A A
ATOM	1150	CE	LYS A 147 LYS A 147	54.835 55.740	7.417 6.291	19.282 19.643	1.00 33.05	Ā
ATOM	1151 1152	NZ C	LYS A 147	52.315	10.743	15.338	1.00 17.25	A
ATOM ATOM	1153	Ö	LYS A 147	52.716	11.320	14.329	1.00 19.15	A
ATOM	1154	N	ILE A 148	51.932	11.391	16.428	1.00 15.47	A
MOTA	1155	CA	ILE A 148	51.969	12.846	16.494	1.00 14.99	A
ATOM	1156	CB	ILE A 148	50.529	13.424	16.642	1.00 15.37	A A
MOTA	1157		2 ILE A 148	50.566 49.689	14.932 13.025	16.740 15.426	1.00 14.06 1.00 16.41	A
MOTA	1158 1159		1 ILE A 148 1 ILE A 148	48.223	13.325	15.550	1.00 18.61	A
MOTA MOTA	1160		ILE A 148	52.829		17.682	1.00 17.07	A
ATOM	1161		ILE A 148	52.721		18.772	1.00 15.61	A
ATOM	1162		SER A 149	53.696		17.458	1.00 16.79	A
MOTA	1163			54.570		18.514	1.00 17.66 1.00 15.95	A A
MOTA	1164			56.042		18.116 19.190		A
MOTA	1165 1166		SER A 149 SER A 149	56.900 54.239		18.763		A
ATOM ATOM	1167		SER A 149	53.854		17.842		A
ATOM	1168		TYR A 150	54.401		20.005		A.
ATOM	1169	CA	TYR A 150	54.085				A
MOTA	1170			52.893		21.310		A A
ATOM	1171			51.679				A
MOTA	1172 1173		1 TYR A 150 1 TYR A 150	50.879 49.733				A
MOTA MOTA	1173		2 TYR A 150	51.313				A
ATOM	1175		2 TYR A 150	50.176		20.901		A
MOTA	1176			49.391	15.957			A
MOTA	1177			48.275				A A
ATOM	1178		TYR A 150	55.237				A
MOTA	1179	0	TYR A 150	55.953	18.207	24.04	2.00 15.05	

MOTA	1180	N	LEU A	151	55.409	20.029	20.649	1.00 17.01	A
MOTA	1181	CA	LEU A		56.449	20.868	21.224	1.00 15.24	A
ATOM	1182	CB	TEO Y		57.540	21.182	20.197	1.00 16.33	A
ATOM	1183	CG	LEU A		58.487	22.335	20.575	1.00 16.27	A
ATOM ATOM	1184 1185		TER Y		59.402 59.315	21.906 22.755	21.706 19.359	1.00 17.13 1.00 19.34	A A
ATOM	1186	C	LEU A		55.825	22.174	21.666	1.00 16.08	A
ATOM	1187	õ	LEU A		55.221	22.881	20.860	1.00 16.22	A
ATOM	1188	N	THR A		55.952	22,497	22.945	1.00 16.84	A
ATOM	1189	CA	THR A	152	55.428	23.765	23.424	1.00 18.70	A
ATOM	1190	CB	THR A	152	55.283	23.799	24.946	1.00 20.14	A
MOTA	1191		THR A		56.576	23.633	25.544	1.00 23.32	A
ATOM	1192		THR A		54.355	22.694	25.419	1.00 18.36	A
ATOM	1193	C	THR A		56.498	24.772	23.050 23.034	1.00 20.04 1.00 20.72	A A
ATOM ATOM	1194 1195	O N	THR A		57.689 56.085	24.448 25.986	22.735	1.00 20.72	A
ATOM	1196	CA	LEU A		57.043	27.014	22.389	1.00 24.69	A
ATOM	1197	CB	LEU A		57.579	26.794	20.960	1.00 24.19	A
ATOM	1198	CG	LEU A		56.716	26.942	19.694	1.00 26.72	A
MOTA	1199	CD1	LEU A	153	55.303	26.451	19.959	1.00 27.32	A
MOTA	1200		LEU A		56.686	28.393	19.249	1.00 26.15	A
MOTA	1201	C	LEU A		56.410	28.385	22.531	1.00 26.36	A
MOTA	1202	0	LEU A		55.180	28.511	22.597	1.00 29.59 1.00 26.29	A A
MOTA	1203 1204	N CA	LEU A		57.262 56.830	29.401 30.787	22.620 22.729	1.00 26.89	A
ATOM	1205	CB	LEU A		57.459	31.444	23.965	1.00 26.94	A
ATOM	1206	CG	LEU A		56.966	32.833	24.407	1.00 28.58	A
ATOM	1207		LEU A		55.507	32.755	24.864	1.00 24.43	A
MOTA	1208	CD2	LEU A	154	57.845	33.342	25.549	1.00 27.14	A
MOTA	1209	C	LEU A	154	57.337	31.458	21.456	1.00 28.94	A
MOTA	1210	0	LEU A		58.538	31.689	21.304	1.00 30.73	A
ATOM	1211	N	PRO A		56.428	31.773	20.518	1.00 30.57 1.00 29.60	A A
ATOM	1212	CD CA	PRO A		54.975 56.806	31.534	20.559 19.254	1.00 25.60	A
MOTA MOTA	1213 1214	CB	PRO A		55.460	32.668	18.581	1.00 30.63	A
ATOM	1215	CG	PRO A		54.612	31.552	19.087	1.00 28.73	A
MOTA	1216	C	PRO A		57.639	33.688	19.370	1.00 33.58	A
MOTA	1217	0	PRO A	. 155	57.322	34.593	20.136	1.00 33.98	A
MOTA	1218	N	SER A		58.706	33.741	18.586	1.00 35.79	A
MOTA	1219	CA	SER A		59.595	34.888	18.546	1.00 37.77	A
ATOM	1220	CB	SER A		60.604	34.839 34.966	19.694 20.949	1.00 38.66 1.00 44.00	A A
MOTA MOTA	1221 1222	OG C	SER A		59.955 60.332	34.841	17.222	1.00 38.83	A
ATOM	1223	ō	SER A		60.257	33.849	16.492	1.00 38.36	A
ATOM	1224	N	ALA A		61.042	35.915	16.909	1.00 40.38	A
ATOM	1225	CA	ALA A	157	61.796	35.972	15.670	1.00 39.93	A
ATOM	1226	CB	ALA A		61.822	37.401	15.148	1.00 40.36	A
ATOM	1227	C	ALA A		63.214	35.466	15.918	1.00 39.65	A
MOTA	1228	0	ALA A		64.05B	35.504	15.021	1.00 39.72 1.00 39.12	A
ATOM ATOM	1229	N CA	GLU A		63.463 64.784	34.984 34.480	17.135 17.517	1.00 40.24	A A
ATOM	1230 1231	CB	GLU A		65.082	34.808	18.988	1.00 44.21	A
ATOM	1232	CG	GLU A		65.426	36.268	19.287	1.00 50.31	A
ATOM	1233	CD	GLU A		64.204	37.174	19.356	1.00 55.36	A
MOTA	1234	OE1	GLU A	158	64.353	38.351	19.765	1.00 55.75	A
ATOM	1235		GLU A		63.095	36.712	19.002	1.00 58.12	A
MOTA	1236	C	GLU A		65.005	32.979	17.303	1.00 38.02	A
MOTA	1237	0	GLU A		66.130 63.950	32.493 32.234	17.419 17.002	1.00 36.30 1.00 35.79	A A
MOTA MOTA	1238 1239	N CA	GLU A		64.136	30.807	16.805	1.00 35.79	A
ATOM	1240	CB	GLU F		63.949	30.066	18.135	1.00 36.97	A
ATOM	1241	CG	GLU A		62.699	30.439	18.891	1.00 41.68	A
ATOM	1242	CD	GLU A		62.717	29.933	20.323	1.00 44.82	A
MOTA	1243		GLU A		62.819	28.705	20.527	1.00 46.62	A
MOTA	1244		GLU A		62.631	30.767	21.248	1.00 47.25	A
MOTA	1245	C	GLU A		63.277	30.162	15.735 15.473	1.00 32.21 1.00 32.05	A A
MOTA MOTA	1246 1247	O N	GLU A		62.147 63.849	30.574 29.147	15.4/3	1.00 32.05	A
ATOM	1247	CA	SER I		63.167	28.394	14.076	1.00 28.89	A
MOTA	1249	CB	SER A		63.885	28.551	12.734	1.00 27.34	A
MOTA	1250	OG	SER A		65.206	28.053	12.807	1.00 29.49	A
ATOM	1251	С	SER A		63.241	26.957	14.565	1.00 27.42	A
MOTA	1252	0		160	64.092	26.628	15.392	1.00 25.45	A
MOTA	1253	N	TYR 1	A 161	62.359	26.101	14.066	1.00 24.73	A

ATOM	1254	CA	TYR	a	161	62.359	24.725	14 517	1 00	24 26	
								14.517		24.26	A
MOTA	1255	CB	TYR			61.172	24.480	15.451		23.50	A
ATOM	1256	CG	TYR			60.935	25.593	16.434		24.01	A
ATOM	1257	CDI	TYR	A	161	60.255	26.748	16.052	1.00	26.02	A
ATOM	1258	CE1	TYR	A	161	60.009	27.774	16.959	1.00	27.93	A
MOTA	1259	CD2	TYR	A	161	61.374	25.491	17.753	1.00	24.78	A
ATOM	1260	CE2	TYR	A	161	61.136	26.514	18.674	1.00	25.93	A
ATOM	1261	CZ	TYR			60.450	27.650	18.270		27.56	A
ATOM	1262	OH	TYR			60.182	28.650	19.173		29.78	A
ATOM	1263	C	TYR			62.330	23.700	13.397		25.15	A
ATOM	1264	0	TYR			62.082	24.021	12.239		24.96	A
MOTA	1265	N	ASP			62.600	22.455	13.775		26.26	A
MOTA	1266	CA	ASP	A	162	62.598	21.331	12.858	1.00	26.94	A
MOTA	1267	CB	ASP	A	162	64.007	21.014	12.356	1.00	30.11	A
ATOM	1268	CG	ASP	A	162	64.548	22.067	11.434	1.00	32.85	A
MOTA	1269	OD1	ASP	A	162	64.075	22.138	10.277		33.31	A
ATOM	1270		ASP			65.443	22.819	11.874		33.08	A
ATOM	1271	C	ASP			62.122	20.117	13.613	-	25.87	A
	1272	ō	ASP								
MOTA						62.449	19.947	14.789		24.38	A
ATOM	1273	N	CYS			61.352	19.277	12.935		23.95	A
ATOM	1274	CA	CYS			60.914	18.027	13.530		24.46	A
MOTA	1275	С	CYS			61.916	17.043	12.938		22.46	A
ATOM	1276	0	CYS	A	163	62.110	17.021	11.726	1.00	24.01	A
ATOM	1277	CB	CYS	A	163	59.497	17.658	13.083	1.00	24.14	A
MOTA	1278	SG	CYS	A	163	58.931	16.101	13.836	1.00	30.35	A
ATOM	1279	N	LYS	Α	164	62.571	16.259	13.782	1.00	22.96	A
ATOM	1280	CA.	LYS			63.559	15.292	13.307		24.69	A
ATOM	1281	CB	LYS			64.867	15.450	14.089		27.54	A
			LYS			65.977		13.689			
ATOM	1282	CG					14.490			28.93	A
ATOM	1283	CD	LYS			67.179	14.643	14.622		32.03	A
MOTA	1284	CE	LYS			68.254	13.596	14.350		33.85	A
MOTA	1285	NZ	Lys			69.319	13.607	15.398	1.00	36.46	A
MOTA	1286	С	LYS	A	164	63.023	13.875	13.463	1.00	24.25	A
ATOM	1287	0	LYS	A	164	62.697	13.443	14.570	1.00	23.52	A
MOTA	1288	N	VAL	A	165	62.931	13.160	12.345	1.00	23.37	A
ATOM	1289	CA	VAL	A	165	62.415	11.797	12.344	1.00	24.06	A
ATOM	1290	СВ	VAL			61.174	11.682	11.408		23.45	A
ATOM	1291		VAL			60.657	10.248	11.382		18.80	A
ATOM	1292		VAL			60.078	12.632	11.878		22.37	A
					165			11.903			A
ATOM	1293	C				63.457	10.772			25.04	
MOTA	1294	0			165	64.103	10.931	10.869		25.12	A
MOTA	1295	N	GLU			63.621	9.725	12.703		26.91	A
ATOM	1296	CA	GLÜ	A	166	64.556	8.648	12.383	1.00	28.84	A
MOTA	1297	CB	GLU	A	166	65.554	8.424	13.523	1.00	30.71	A
ATOM	1298	CG	GTA	A	166	66.382	9.634	13.922	1.00	36.90	A
ATOM	1299	CD	GLU	A	166	67.247	9.356	15.147	1.00	39.97	A
ATOM	1300	OE1	GLU	А	166	67.466	10.286	15.954	1.00	43.02	A
ATOM	1301		GLU			67.714	8.206	15.301		43.24	A
ATOM	1302	C	GLU			63.739	7.369	12.183		28.96	A
ATOM	1303	ō			166	62.975	6.971	13.067		27.40	A
	1304	И					6.728	11.029		29.87	A
ATOM					167	63.910					
ATOM	1305	CA			167	63.189	5.496	10.713		30.70	A
ATOM	1306	CB			167	61.838	5.833	10.084		30.90	A
MOTA	1307	CG			167	60.932	4.655	9.933		34.01	A
ATOM	1308		HIS			60.698	3.842	8.876		33.60	A
ATOM	1309	ND1	HIS	A	167	60.159	4.172	10.967	1.00	36.69	A
ATOM	1310	CE1	HIS	Α	167	59.488	3.112	10.554	1.00	34.84	A
MOTA	1311	NE2	HIS	A	167	59.798	2.890	9.290	1.00	34.90	A
ATOM	1312	C			167	63.999	4.639	9.739		31.21	A
MOTA	1313	ō			167	64.696	5.167	8.866		29.44	A
MOTA	1314	N			168	63.895	3.320	9.879		31.70	A
ATOM	1315	CA			168	64.625	2.402	9.006		31.76	A
MOTA	1316	CB			168	64.344	0.954	9.396		30.39	A
ATOM	1317	CG			168	64.735	0.650	10.797		28.49	A
MOTA	1318		TRP			64.115	-0.297	11.666		28.31	A
MOTA	1319	CE2	TRP	A	168	64.837	-0.288	12.878	1.00	28.31	A
ATOM	1320	CE3	TRP	A	168	63.017	-1.157	11.538	1.00	26.47	A
ATOM	1321	CD1	TRP	A	168	65.778	1.184	11.491	1.00	28.32	A
MOTA	1322		TRP			65.849	0.627	12.744	1.00	28.98	A
ATOM	1323		TRP			64.498	-1.107	13.958		28.85	A
ATOM	1324		TRP			62.678	-1.970	12.608		27.57	A
MOTA	1325		TRP			63.418	-1.940	13.805		29.20	A
ATOM	1326	C			168			7.523		33.06	A
						64.332	2.588				
ATOM	1327	0	IKP	A	168	65.190	2.314	6.682	1.00	32.28	A

ATOM	1328	N	GLY A 1	69 63.126	3.049	7.202	1.00 34.81	A
MOTA	1329	CA	GLY A 1		3.263	5.810	1.00 35.23	A
MOTA	1330	C	GLY A 1		4.588	5.266	1.00 37.25	A
ATOM	1331	0	GLY A 1		4.992 5.268	4.162 6.049	1.00 37.65 1.00 39.27	A A
ATOM ATOM	1332 1333	N CA	LEU A 1		6.555	5.660	1.00 39.27	A
ATOM	1333	CB	LEU A 1		7.626	6.706	1.00 38.47	A
ATOM	1335	CG	LEU A 1		8.143	6.843	1.00 38.66	A
ATOM	1336	CD1			8.919	8.142	1.00 37.48	A
MOTA	1337	CD2	LEU A 1	70 62.572	9.017	5.653	1.00 37.65	A
ATOM	1338	С	LEU A 1		6.425	5.556	1.00 43.62	A
MOTA	1339	0	LEU A 1		5.762	6.382	1.00 44.45 1.00 46.98	A
ATOM	1340	n Ca	ASP A 1 ASP A 1		7.066 7.036	4.545 4.350	1.00 48.99	A A
MOTA MOTA	1341 1342	CB	ASP A 1		7.810	3.086	1.00 51.12	A
ATOM	1343	CG	ASP A 1		7.466	1.895	1.00 53.30	A
ATOM	1344		ASP A 1	71 66.520	7.761	1.936	1.00 54.82	A
MOTA	1345	OD2	ASP A 1	71 68.271	6.903	0.917	1.00 54.86	A
MOTA	1346	C	ASP A 1		7.726	5.554	1.00 48.82	A
ATOM	1347	0	ASP A 1		7.093	6.420	1.00 48.88	A
ATOM	1348	N	LYS A 1		9.044 9.877	5.585 6.659	1.00 48.96 1.00 48.79	A A
ATOM ATOM	1349 1350	CA CB	LYS A 1		11.059	6.084	1.00 51.32	A
ATOM	1351	CG	LYS A 1		10.698	5.075	1.00 55.53	A
MOTA	1352	CD	LYS A 1		11.952	4.571	1.00 57.81	A
MOTA	1353	CE	LYS A 1	.72 72.859	11.621	3.518	1.00 59.22	A
MOTA	1354	NZ	LYS A 1		10.702	4.038	1.00 58.32	A
ATOM	1355	C	LYS A 1		10.419	7.420	1.00 46.36 1.00 44.39	A A
ATOM	1356 1357	o N	LYS A 1 PRO A 1		10.381 10.920	6.919 8.645	1.00 44.39	A
ATOM ATOM	1358	CD	PRO A 1		10.866	9.469	1.00 44.15	A
ATOM	1359	CA	PRO A 1		11.462	9.410	1.00 42.74	A
MOTA	1360	CB	PRO A 1	.73 67.768	12.050	10.637	1.00 42.02	A
MOTA	1361	CG	PRO A 1		11.080	10.872	1.00 44.25	A
MOTA	1362	C	PRO A 1		12.517	8.578	1.00 41.09	A
ATOM	1363	0	PRO A 1		13.309 12.502	7.877 8.636	1.00 39.67 1.00 39.80	A A
ATOM ATOM	1364 1365	N CA	LEU A 1		13.457	7.888	1.00 38.58	A
ATOM	1366	CB	LEU A 1		12.838	7.522	1.00 38.73	A
MOTA	1367	CG	LEU A 1	L74 62.202	13.329	6.251	1.00 39.18	A
ATOM	1368	CD1	LEU A 1		12.691	6.170	1.00 39.20	A
MOTA	1369		LEU A 1		14.836	6.245	1.00 40.87	A A
MOTA	1370	C	LEU A 1		14.662 14.514	8.785 9.943	1.00 37.43 1.00 37.68	A
MOTA MOTA	1371 1372	Ŋ	LEU A 1		15.849	8.255	1.00 35.85	A
ATOM	1373	CA	LEU A 1		17.077	9.012	1.00 34.38	A
ATOM	1374	CB	LEU A 1	L75 65.400	17.882	9.074	1.00 33.21	A
ATOM	1375	CG	LEU A 3		17.502	10.147	1.00 34.82	A
ATOM	1376		LEUAI		17.768	11.526	1.00 34.32	A
ATOM	1377	CD2	LEU A 1		16.038 17.898	10.008 8.337	1.00 35.37 1.00 33.09	A A
MOTA MOTA	1378 1379	0	LEU A		18.137	7.132	1.00 33.84	A
ATOM	1380	N	LYS A		18.312	9.108	1.00 30.14	A
ATOM	1381	CA	LYS A		19.119	8.566	1.00 30.03	A
MOTA	1382	CB	LYS A		18.416	8.772	1.00 30.60	A
MOTA	1383	CG	LYS A		19.049	8.010	1.00 33.60	A
MOTA	1384 1385	CD	LYS A :		19.054 17.642	6.508 5.960	1.00 37.73 1.00 37.37	A A
ATOM ATOM	1386	CE NZ	LYS A		17.629	4.484	1.00 41.15	A
ATOM	1387	c	LYS A		20.457	9.292	1.00 28.62	A
ATOM	1388	0	LYS A		20.524	10.501	1.00 27.68	A
ATOM	1389	N	HIS A		21.520	8.539	1.00 28.72	A
MOTA	1390	CA	HIS A		22.868	9.088	1.00 29.54	A
MOTA	1391		HIS A		23.691	8.195 8.663	1.00 29.51 1.00 30.53	A A
ATOM	1392 1393		HIS A :			8.114	1.00 30.33	A
MOTA MOTA	1394		l HIS A			9.849	1.00 32.09	A
ATOM	1395		1 HIS A			10.010	1.00 32.65	A
ATOM	1396		2 HIS A	177 62.542		8.971	1.00 32.04	A
MOTA	1397		HIS A			9.304	1.00 29.24	A
MOTA	1398		HIS A			8.549	1.00 27.66 1.00 30.09	A A
MOTA MOTA	1399 1400		TRP A			10.340 10.674	1.00 30.03	A
ATOM	1401					11.632	1.00 28.07	A
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ATOM	1402	CG	TRP :	A.	178	56.681	25.422	11.851	1.00	25.25	A
MOTA	1403	CD2	TRP 2	A	178	56.476	26.518	12.761	1.00	21.68	A
ATOM	1404	CE2	TRP :	A	178	55.138	26.942	12.611	1.00	20.86	A
ATOM	1405		TRP			57.292	27.178	13.688		20.72	A
							25.239	11.206		24.81	A
ATOM	1406		TRP .			55.489					
ATOM	1407	NEI	TRP .			54.559	26.146	11.657		21.51	A
ATOM	1408	CZ2	TRP .	A	178	54.598	27.999	13.354	1.00	21.11	A
ATOM	1409	CZ3	TRP .	A	178	56.754	28.229	14.428	1.00	21.58	A
ATOM	1410		TRP .	A	178	55.419	28.627	14.255	1.00	20.94	A
			TRP			59.425	26.628	11.348		36.30	A
ATOM	1411	С									A
ATOM	1412	0	TRP			60.314	26.591	12.195		36.91	
MOTA	1413	N	GLU	A	179	58.852	27.761	10.975	1.00	40.65	A
MOTA	1414	CA	GLU .	A	179	59.240	29.029	11.587	1.00	45.62	A
MOTA	1415	CB	GLU .	A	179	60.481	29.622	10.899	1.00	47.42	A
ATOM	1416	CG	GLU			60.323	29.868	9.404	1.00	52.77	A
							30.624	8.806		55.17	A
MOTA	1417	CD	GLU			61.498					
MOTA	1418	OE1	GLU			62.653	30.179	8.987		57.20	A
ATOM	1419	OE2	GLU	A	179	61.265	31.663	8.149	1.00	57.21	A
ATOM	1420	C	GLU	A	179	58.074	30.001	11.489	1.00	46.47	A
ATOM	1421	0	GLU	A	179	57.322	29.983	10.513	1.00	45.49	A
			PRO			57.898	30.855	12.509		47.97	A
ATOM	1422	N									A
ATOM	1423	CD	PRO			58.679	31.008	13.752		48.35	
ATOM	1424	CA	PRO	А	180	56.789	31.810	12.460		49.45	A
MOTA	1425	CB	PRO	A	180	56.763	32.372	13.880	1.00	49.39	A
ATOM	1426	CG	PRO	А	180	58,214	32.358	14.266	1.00	48.65	A
ATOM	1427	C	PRO			57.014	32.891	11.401	1.00	50.21	. A
						58.174	33.041	10.950		49.95	A
MOTA	1428	0	PRO							50.90	A
MOTA	1429	OXT	PRO	A		56.030	33.578	11.043			
ATOM	1430	CB	SER	В	3	67.953	-2.426	7.203		59.72	В
ATOM	1431	OG	SER	В	3	68.517	-3.384	6.321	1.00	60.71	В
ATOM	1432	С	SER	В	3	68.164	-3.822	9.277	1.00	57.49	В
ATOM	1433	ō	SER		3	68.117	-4.879	8.642	1.00	57.32	В
							-2.418	8.486		59.35	В
ATOM	1434	N	SER		3	70.072					В
MOTA	1435	CA	SER		3	68.586	-2.517	8.597		58.84	
MOTA	1436	N	PRO	В	4	67.855	-3.763	10.585		55.71	В
MOTA	1437	CD	PRO	В	4	67.914	-2.580	11.463	1.00	54.97	В
ATOM	1438	CA	PRO	в	4	67.438	-4.952	11.338	1.00	53.72	В
ATOM	1439	CB	PRO		4	67.457	-4.467	12.787	1.00	54.71	В
						67.095	-3.021	12.660		54.93	В
MOTA	1440	CG	PRO		4						В
MOTA	1441	С	PRO		4	66.069	-5.487	10.918		51.05	
MOTA	1442	0	PRO	В	4	65.240	-4.753	10.379		50.96	В
MOTA	1443	N	GLU	В	5	65.843	-6.773	11.165	1.00	47.90	В
ATOM	1444	CA	GLU	В	5	64.581	-7.410	10.810	1.00	45.24	В
ATOM	1445	СВ	GTO		5	64.811	-8.893	10.489	1.00	48.23	В
						65.603	-9.656	11.545		54.54	В
MOTA	1446	CG	GLU		5					57.83	В
ATOM	1447	CD	GLU		5		-11.102	11.140			
MOTA	1448	OE1	GLU	В	5	66.421	-11.317	10.024		59.67	В
MOTA	1449	OE2	GLU	В	5	65.609	-12.020	11.941	1.00	59.33	В
ATOM	1450	C	GLU	В	5	63.548	-7.269	11.920	1.00	40.85	В
ATOM	1451	ō	GLU		5	63.876	-7.328	13.105	1.00	40.81	В
					6	62.294	-7.083	11.532	1 00	36.03	В
ATOM	1452	N	ASP								В
ATOM	1453	CA	ASP		6	61.223	-6.936	12.508		32.11	
MOTA	1454	CB	ASP			60.833	-5.460	12.616		29.96	В
ATOM	1455	CG	ASP	В	6	59.933	-5.171	13.798	1.00	27.91	В
ATOM	1456	ODI	. ASP	В	6	59.280	-4.110	13.785	1.00	29.62	В
ATOM	1457		ASP			59.884		14.745	1.00	29.86	В
						60.014		12.077		29.68	В
MOTA	1458	C	ASP							29.14	В
MOTA	1459	0	ASP			59.676		10.899			
ATOM	1460	N	PHE	В	7	59.380		13.032		27.77	В
ATOM	1461	CA	PHE	В	7	58.193	-9.249	12.765	1.00	28.11	В
ATOM	1462	CB	PHE	В	7	58.453	-10.704	13.161	1.00	29.55	В
ATOM	1463	CG	PHE				-11.385	12.282	1.00	31.06	В
							-11.766	10.989		29.85	В
MOTA	1464		PHE							32.21	В
MOTA	1465		2 PHE				-11.603	12.730			
ATOM	1466	CE:	L PHE	E	7		-12.355	10.145		33.75	В
ATOM	1467	CE	2 PHE	E	. 7	61.719	-12.190	11.897		34.27	В
ATOM	1468	CZ	PHE			61.373	-12.568	10.599	1.00	33.07	В
ATOM	1469		PHE			57.032		13.562	1.00	26.58	В
ATOM	1470		PHE			57.046		14.794		25.72	В
						56.023		12.849		25.17	В
MOTA	1471		VAL							23.46	В
MOTA	1472		VAL			54.891		13.493			
MOTA	1473		VAL			54.670				21.55	В
MOTA	1474	CG	1 VAL	E	3 8	53.573				21.83	В
MOTA	1475		2 VAI			55.975	-5.342	12.895	1.00	21.30	В
			,	_	_						

ATOM	1476	C	VAL	я	8	53.556	-8.255	13.467	1.00 24.08	В
ATOM	1477	ō	VAL		8	53.204	-8.912	12.491	1.00 23.46	В
ATOM	1478	N	TYR		9	52.804	-8.127	14.554	1.00 23.26	В
ATOM	1479	CA	TYR		9	51.493	-8.747	14.619	1.00 23.18	В
ATOM	1480	СВ	TYR		9	51.510	-9.978	15.520	1.00 23.12	В
ATOM	1481	CG	TYR		9		-10.786	15.465	1.00 24.54	В
ATOM	1482		TYR		9	50.158	-11.962 ·	14.722	1.00 26.50	В
MOTA	1483	CE1	TYR	В	9	49.000	-12.743	14.716	1.00 25.08	В
MOTA	1484	CD2	TYR	В	9	49.108	-10.399	16.190	1.00 22.88	В
MOTA	1485	CE2	TYR	В	9	47.948	-11.165	16.188	1.00 23.91	В
ATOM	1486	CZ	TYR	В	9	47.902	-12.342	15.455	1.00 24.87	В
ATOM	1487	OH	TYR	В	9	46.780	-13.140	15.501	1.00 25.45	В
ATOM	1488	C	TYR	В	9	50.509	-7.723	15.163	1.00 21.33	В
ATOM	1489	0	TYR	В	9	50.798	-7.028	16.133	1.00 22.92	В
MOTA	1490	N	GLN	В	10	49.353	-7.622	14.521	1.00 19.98	В
MOTA	1491	CA	GLN	В	10	48.326	-6.687	14.952	1.00 19.52	В
MOTA	1492	CB	GLN	В	10	48.171	-5.523	13.962	1.00 19.13	В
ATOM	1493	CG	GLN	В	10	49.433	-4.810	13.509	1.00 19.33	В
ATOM	1494	CD	GLN	В	10	49.117	-3.708	12.499	1.00 17.96	В
ATOM	1495		GI'N		10	48.336	-2.802	12.783	1.00 18.49	В
MOTA	1496		GI'N		10	49.715		11.316	1.00 19.41	В
ATOM	1497	C	GIM		10	46.967	-7.375	15.029	1.00 19.74	В
ATOM	1498	0	GFM		10	46.626	-8.227	14.192	1.00 18.98	В
ATOM	1499	N	PHE		11	46.195	-6.996	16.040	1.00 19.06	В
ATOM	1500	CA	PHE		11	44.842	-7.487	16.182	1.00 16.54	В
ATOM	1501	СВ	PHE		11	44.668	-8.454	17.336	1.00 17.48	В
ATOM	1502	CG	PHE		11	43.237	-8.847	17.544	1.00 16.17	В
ATOM	1503		PHE		11	42.570	-9.604	16.582	1.00 17.49	В
ATOM	1504		PHE		11	42.536	-8.406	18.656	1.00 14.41	В
MOTA	1505		PHE		11	41.219	-9.913	16.725	1.00 18.03	В
ATOM	1506		PHE		11	41.191	-8.708	18.814	1.00 16.34	B
MOTA	1507	cz	PHE		11	40.528	-9.463	17.845 16.450	1.00 17.80	B
MOTA	1508	C	PHE		11	43.984	-6.271 -E E06			В
ATOM	1509	0	PHE		11	44.241	-5.506	17.386	1.00 15.63	В
ATOM	1510	N	LYS		12 12	42.961	-6.094 -4.958	15.625 15.770	1.00 17.63	В
ATOM	1511	CA	LYS		12	42.082 42.188	-4.067	14.536	1.00 17.03	В
MOTA	1512	CB CG	LYS		12	43.599	-3.642	14.192	1.00 15.90	В
ATOM ATOM	1513 1514	CD	LYS		12	43.602	-2.909	12.871	1.00 17.33	В
ATOM	1515	CE	LYS		12	44.946	-2.297	12.570	1.00 18.72	В
ATOM	1516	NZ	LYS		12	44.838	-1.450	11.340	1.00 20.93	В
ATOM	1517	C	LYS		12	40.632	-5.387	15.968	1.00 18.92	В
ATOM	1518	ō	LYS		12	40.041	-6.050	15.109	1.00 17.25	В
MOTA	1519	N	GLY		13	40.076	-5.002	17.114	1.00 17.59	В
MOTA	1520	CA	GLY		13	38.701	-5.322	17.430	1.00 19.88	В
MOTA	1521	c	GLY		13	37.874	-4.113	17.064	1.00 20.12	В
ATOM	1522	ō	GLY		13	37.515	-3.309	17.923	1.00 21.08	В
ATOM	1523	N	MET		14	37.561	-4.000	15.779	1.00 20.42	В
ATOM	1524	CA	MET		14	36.817	-2.866	15.262	1.00 22.96	В
ATOM	1525	CB	MET	В	14	37.334	-2.554	13.866	1.00 23.02	В
ATOM	1526	CG	MET		14	38.846	-2.485	13.820	1.00 23.58	В
ATOM	1527	SD	MET	В	14	39.449	-2.095	12.191	1.00 26.23	В
ATOM	1528	CE	MET	В	14	39.260	-0.318	12.182	1.00 25.78	В
ATOM	1529	C	MET	В	14	35.295	-2.997	15.242	1.00 23.12	В
ATOM	1530	0	MET	В	14	34.751	-4.089	15.081	1.00 24.36	В
ATOM	1531	N	CYS	В	15	34.628	-1.860	15.427	1.00 24.04	В
MOTA	1532	CA	CYS	В	15	33.173	-1.768	15.433	1.00 24.91	В
MOTA	1533	C	CYS	В	15	32.808	-0.587	14.547	1.00 25.49	В
MOTA	1534	0	CYS	В	15	33.369	0.504	14.700	1.00 23.97	В
ATOM	1535	CB	CYS		15	32.630	-1.489	16.847	1.00 26.02	В
ATOM	1536	SG	CYS		15	32.691		18.084	1.00 33.69	В
MOTA	1537	N	TYR		16	31.871	-0.805	13.630	1.00 25.87	В
MOTA	1538	CA	TYR		16	31.413	0.244	12.724	1.00 25.59	В
MOTA	1539	CB	TYR		16	31.539	-0.223	11.274	1.00 24.73	В
MOTA	1540	CG	TYR		16	32.958	-0.575	10.879	1.00 26.05	В
MOTA	1541		TYR		16	33.523	-1.795	11.239	1.00 22.96	В
MOTA	1542		TYR		16	34.843		10.904	1.00 25.81	В
MOTA	1543		TYR		16	33.748		10.171	1.00 25.30	B
MOTA	1544		TYR		16	35.066		9.835	1.00 25.12	В
MOTA	1545	CZ	TYR		16	35.607		10.202	1.00 26.66 1.00 29.22	В
ATOM	1546	OH	TYR		16	36.908		9.868 13.045	1.00 25.22	В
MOTA MOTA	1547 1548	C	TYR		16	29.960 29.113		13.045	1.00 26.41	В
ATOM	1548	И О	TYR		16 17	29.113		13.266	1.00 27.76	В
2. C.	*343	74	FILE		11	25.00%	1.000	20.200	2.00 27.70	_

ATOM	1550	CA	PHE	В	17	28.346	2.338	13.613	1.00 29.09	В
MOTA	1551	CB	PHE	В	17	28.382	3.047	14.967	1.00 28.08	В
ATOM	1552	CG	PHE		17	28.885	2.194	16.091	1.00 28.21	В
MOTA	1553	CD1			17	28.056	1.253	16.693	1.00 27.20	В
MOTA	1554	CD2			17	30.188	2.340	16.558	1.00 26.60	В
ATOM	1555	CE1			17	28.519	0.470	17.752	1.00 28.13 1.00 25.62	B B
ATOM	1556	CE2	PHE		17	30.662	1.565 0.629	17.610 18.210	1.00 25.62	В
MOTA	1557	.cz	PHE		17 17	29.828 27.772	3.318	12.592	1.00 30.71	В
MOTA MOTA	1558 1559	C 0	PHE		17	28.452	4.239	12.155	1.00 31.05	В
ATOM	1560	И	THR		18	26.506	3.125	12.237	1.00 33.51	В
ATOM	1561	CA	THR		18	25.831	4.005	11.291	1.00 36.95	В
ATOM	1562	СВ	THR		18	25.797	3.395	9.875	1.00 37.23	В
ATOM	1563	OG1	THR	В	18	27.133	3.105	9.447	1.00 40.77	В
ATOM	1564	CG2	THR	В	18	25.171	4.369	8.891	1.00 38.43	В
MOTA	1565	C	THR	В	18	24.398	4.273	11.753	1.00 38.56	В
MOTA	1566	0	THR		18	23.671	3.351	12.131	1.00 38.36	В
MOTA	1567	N	ASN		19	24.007	5.544	11.726	1.00 39.80	В
MOTA	1568	CA	ASN		19	22.668	5.961	12.132 11.110	1.00 41.35	B
MOTA	1569	CB	ASN		19	21.638	5.465 6.190	11.223	1.00 42.85	В
MOTA	1570	CG	asn asn		19 19	20.311 20.271	7.378	11.548	1.00 42.24	В
ATOM ATOM	1571 1572		ASN		19	19.219	5.485	10.937	1.00 42.57	В
ATOM	1573	C	ASN		19	22.352	5.416	13.521	1.00 42.37	В
ATOM	1574	ō	ASN		19	21.540	4.503	13.673	1.00 43.36	В
ATOM	1575	N	GLY		20	22.997	5.989	14.533	1.00 42.56	В
ATOM	1576	CA	GLY	В	20	22.790	5.535	15.894	1.00 43.89	В
ATOM	1577	C	GLY		20	23.293	4.110	16.031	1.00 45.10	В
MOTA	1578	0	GLY		20	24.421	3.807	15.646	1.00 44.28	В
MOTA	1579	N	THR		21	22.458	3.232	16.575	1.00 46.37	B B
ATOM	1580	CA	THR		21	22.824	1.832 1.373	16.738 18.199	1.00 47.42 1.00 48.57	В
ATOM	1581	CB	THR		21 21	22.667 21.438	1.885	18.731	1.00 49.14	В
ATOM ATOM	1582 1583	CG2			21	23.843	1.856	19.043	1.00 47.59	В
ATOM	1584	C	THR		21	21.958	0.947	15.846	1.00 48.74	В
ATOM	1585	ō	THR		21	21.925	-0.276	16.016	1.00 48.04	В
MOTA	1586	N	GLU	В	22	21.253	1.570	14.902	1.00 48.57	В
MOTA	1587	CA	GLU	В	22	20.405	0.822	13.979	1.00 48.90	В
ATOM	1588	CB	GLU		22	19.741	1.745	12.957	1.00 52.60	B
ATOM	1589	CG	GLU		22	18.669	2.667 3.297	13.493 12.368	1.00 58.06 1.00 62.27	B
MOTA	1590	CD	GLU		22 22	17.862 17.027	4.185	12.648	1.00 63.99	В
ATOM ATOM	1591 1592		GLU		22	18.065	2.894	11.199	1.00 64.70	В
ATOM	1593	c	GLU		22	21.285	-0.156	13.229	1.00 46.38	В
ATOM	1594	0	GLU		22	21.029	-1.356	13.209	1.00 45.52	В
MOTA	1595	N	ARG	В	23	22.324	0.379	12.601	1.00 45.42	В
MOTA	1596	CA	ARG		23	23.260	-0.438	11.844	1.00 44.59	В
ATOM	1597	CB	ARG		23	23.423	0.127	10.422 9.554	1.00 45.69 1.00 49.95	B
MOTA	1598	CG	ARG		23	22.169 22.406	-0.062 0.237	8.074	1.00 53.34	В
MOTA	1599 1600	CD NE	ARG		23 23	22.153	1.632	7.708	1.00 55.57	В
ATOM ATOM	1601	CZ	ARG		23	20.949	2.200	7.700	1.00 57.20	В
ATOM	1602		ARG		23	19.878	1.495	8.042	1.00 58.09	В
ATOM	1603		ARG		23	20.813	3.471	7.340	1.00 56.82	В
ATOM	1604	C	ARG	В	23	24.606	-0.534	12.567	1.00 40.56	В
MOTA	1605	0	ARG		23	25.306	0.459	12.748	1.00 41.15	В
MOTA	1606	N	VAI			24.944	-1.743	12.995	1.00 38.17 1.00 34.88	B B
MOTA	1607	CA	VAI		24	26.191 25.931	-1.996 -2.314	13.708 15.200	1.00 34.41	В
MOTA	1608	CB	VAI VAI			27.251	-2.526	15.918	1.00 35.28	В
MOTA MOTA	1609 1610		VAL			25.146	-1.190	15.852	1.00 34.70	В
ATOM	1611	C	VAI			26.909	-3.194	13.100	1.00 32.34	В
ATOM	1612	ō	VAI			26.287	-4.214	12.812	1.00 33.23	В
MOTA	1613	N	ARC			28.217	-3.076	12.898	1.00 30.18	В
ATOM	1614	CA	ARC	3 B	25	28.970	-4.194	12.354	1.00 26.97	В
ATOM	1615	СВ	ARG	3 B	25	29.225	-4.022	10.852	1.00 27.67	В
ATOM	1616	CG	ARG			29.400	-5.362	10.170	1.00 29.58 1.00 31.26	B
MOTA	1617	CD		3 B		30.406 30.058	-5.363 -4.454	9.052 7.974	1.00 31.26	В
ATOM ATOM	1618 1619	NE		3 B 3 B		30.415	-4.631	6.705	1.00 33.22	В
ATOM	1619	CZ NH	ARG 1 ARG			31.124	-5.695	6.346	1.00 31.13	В
MOTA	1621		2 AR			30.087	-3.726	5.799	1.00 30.62	В
ATOM	1622			3 E		30.305	-4.402		1.00 24.10	В
MOTA	1623	0	AR	G E	25	31.095	-3.477	13.225	1.00 22.56	В

ATOM	1624	N	LEU	В	26	30.551	-5.630	13.495	1.00 22.65	В
ATOM	1625	CA	LEU	В	26	31.801	-5.942	14.163	1.00 22.38	В
MOTA	1626	CB	LEU		26	31.558	-6.888	15.345	1.00 20.25	В
ATOM	1627	CG	LEU	В	26	32.795	-7.389	16.100	1.00 19.86	В
MOTA	1628	CD1	LEU	B	26	32.452	-7.613	17.568	1.00 22.49	В
MOTA	1629	CDZ	LEU		26	33.304	-8.665	15.464	1.00 18.43	В
ATOM	1630	C	LEU	В	26	32.726	-6.591	13.150	1.00 21.50	В
ATOM	1631	0	LEU	R	26	32.289	-7.402	12.342	1.00 22.83	В
MOTA	1632	N	VAL	В	27	33.998	-6.208	13.177	1.00 21.29	В
MOTA	1633	CA	VAL	В	27	34.984	-6.780	12.270	1.00 20.66	В
			VAL		27	35.178	-5.911	11.004	1.00 20.59	В
MOTA	1634	CB								
ATOM	1635	CG1	VAL	В	27	36.169	-6.576	10.069	1.00 19.45	В
ATOM	1636	CG2	VAL	В	27	33.849	-5.696	10.297	1.00 22.37	В
							-6.885	12.988	1.00 22.39	В
ATOM	1637	C	VAL		27	36.330				
ATOM	1638	0	VAL	В	27	37.046	-5.889	13.135	1.00 22.63	В
ATOM	1639	N	SER	В	28	36.673	-8.083	13.450	1.00 21.32	В
									1.00 21.51	В
ATOM	1640	CA	SER	B	28	37.947	-8.259	14.130		
ATOM	1641	CB	SER	В	28	37.831	-9.284	15.275	1.00 19.72	В
ATOM	1642	OG	SER	R	28	37 542	-10.581	14.819	1.00 24.33	В
ATOM	1643	C	SER	В	28	38.954	-8.693	13.074	1.00 21.25	В
ATOM	1644	0	SER	В	28	38.661	-9.537	12.229	1.00 19.44	В
		N	ARG		29	40.137	-8.089	13.106	1.00 20.61	В
ATOM	1645									
ATOM	1646	CA	ARG	В	29	41.158	-8.402	12.115	1.00 19.66	В
ATOM	1647	CB	ARG	В	29	41.418	-7.169	11.230	1.00 19.91	В
			ARG		29	40.178	-6.407	10.754	1.00 16.79	В
ATOM	1648	CG								
ATOM	1649	CD	ARG	В	29	40.608	-5.121	10.031	1.00 18.10	В
ATOM	1650	NE	ARG	В	29	39.487	-4.318	9.553	1.00 19.38	В
			ARG			38.738	-4.619	8.497	1.00 20.62	В
MOTA	1651	CZ			29					
ATOM	1652	NH1	ARG	В	29	38.983	-5.714	7.789	1.00 19.50	В
ATOM	1653	NH2	ARG	В	29	37.736	-3.822	8.149	1.00 21.90	В
						42.482	-8.833	12.738	1.00 18.57	В
MOTA	1654	C	ARG		29					
MOTA	1655	0	ARG	В	2 9	43.024	-8.121	13.584	1.00 19.40	В
ATOM	1656	N	SER	В	30	42.991	-9.995	12.326	1.00 18.99	В
							-10.501	12.797	1.00 21.66	В
MOTA	1657	CA	SER		30					
ATOM	1658	СВ	SER	В	30	44.241	-12.015	13.023	1.00 22.77	В
MOTA	1659	OG	SER	В	30	43.390	-12.352	14.106	1.00 26.81	В
							-10.163	11.673	1.00 23.37	В
ATOM	1660	С	SER		30					
ATOM	1661	0	SER	В	30	45.055	-10.553	10.522	1.00 21.31	В
ATOM	1662	N	ILE	В	31	46.338	-9.450	12.009	1.00 24.76	В
										В
ATOM	1663	CA	ILE	B	31	47.298	-8.998	10.999	1.00 24.33	
MOTA	1664	CB	ILE	В	31	47.341	-7.440	10.958	1.00 25.20	В
	1665		ILE		31	47.982	-6.964	9.672	1.00 23.24	В
MOTA										
ATOM	1666	CG1	ILE	В	31	45.934	-6.857	11.106	1.00 26.96	В
MOTA	1667	CD1	ILE	В	31	45.032	-7.136	9.947	1.00 31.25	В
					31	48.741	-9.460	11.187	1.00 23.98	В
ATOM	1668	С	IFE							
MOTA	1669	0	ILE	В	31	49.298	-9.318	12.272	1.00 22.29	В
MOTA	1670	N	TYR	В	32	49.345	-9.993	10.123	1.00 25.50	В
					32		-10.405	10.162	1.00 26.21	В
ATOM	1671	CA	TYR							
MOTA	1672	CB	TYR	В	32	50.965	-11.764	9.492	1.00 28.46	В
ATOM	1673	CG	TYR	В	32	52.406	-12.224	9.544	1.00 31.10	В
			TYR		32		-12.412	10.765	1.00 32.47	В
MOTA	1674									
MOTA	1675	CB1	TYR	В	32	54.393	-12.780		1.00 34.69	В
MOTA	1676	CD2	TYR	В	32	53.140	-12.424	8.375	1.00 33.60	В
							-12.795	8.422	1.00 34.50	В
MOTA	1677		TYR		32					
MOTA	1678	\mathbf{cz}	TYR	В	32	55.103	-12.965	9.654	1.00 35.65	В
MOTA	1679	OH	TYR	В	32	56.438	-13.281	9.717	1.00 37.73	В
					32	51.478		9.384	1.00 25.67	В
MOTA	1680	C	TYR							
MOTA	1681	0	TYR	В	32	51.273	-9.140	8.174	1.00 24.75	В
ATOM	1682	N	ASN	В	33	52.319	-8.559	10.094	1.00 25.63	В
					33	53.036		9.526	1.00 24.95	В
MOTA	1683	CA	asn							
MOTA	1684	СВ	asn	В	33	53.955	-7.848	8.379	1.00 23.75	В
MOTA	1685	CG	ASN	В	33	55.171	-8.615	8.878	1.00 24.11	В
			ASN			55.803		9.861	1.00 25.42	В
MOTA	1686				33					
ATOM	1687	ND2	: ASN	В	33	55.506	-9.708	8.204	1.00 25.18	В
ATOM	1688	C	ASN		33	51.990	-6.392	9.070	1.00 25.11	В
								9.893	1.00 26.06	В
MOTA	1689	0	asn		33	51.491				
MOTA	1690	'N	ARG	B.	34	51.652	-6.375	7.786	1.00 25.75	В
MOTA	1691	CA	ARG		34	50.631	-5.449	7.296	1.00 27.64	В
									1.00 27.74	В
MOTA	1692	CB	ARG		34	51.244		6.408		
MOTA	1693	CG	ARG	B	34	51.972	-3.257	7.158	1.00 29.94	В
ATOM	1694	CD	ARG		34	51.664		6.541	1.00 32.95	В
MOTA	1695	NE	ARG	B	34	51.897		5.101	1.00 35.17	В
MOTA	1696	CZ	ARG	В	34	51.392	-0.973	4.267	1.00 37.51	В
ATOM			L ARG		34	50.622		4.729	1.00 39.45	В
25 V Old	1697	MIL.	- 446		J-2	30.022				_

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MOTA	1698	NH2	ARG	В	34	51.642	-1.058	2.967	1.00 36.90	В
MOTA	1699	C	ARG	В	34	49.587	-6.218	6.498	1.00 26.48	В
MOTA	1700	0	ARG	В	34	48.740	-5.639	5.825	1.00 27.17	В
ATOM	1701	N	GLU		35	49.647	-7.534	6.602	1.00 25.66	В
									1.00 26.99	В
MOTA	1702	CA	GLU		35		-8.394	5.867		
MOTA	1703	СВ	GLU	В	35	49.570	-9.483	5.175	1.00 31.53	В
MOTA	1704	CG	GLU	В	35	48.814	-10.396	4.235	1.00 36.29	В
MOTA	1705	æ	GLU	В	35	49.695	-11.530	3.731	1.00 40.61	В
			GLU				-11.240	3.276	1.00 45.20	В
MOTA	1706				35					
MOTA	1707	OE2	GLU	В	35	49.266	-12.705	3.791	1.00 41.13	В
ATOM	1708	С	GLU	В	35	47.699	-9.031	6.764	1.00 25.09	В
MOTA	1709	0	GLU	В	35	48.028	-9.807	7.663	1.00 23.31	В
ATOM	1710	N	GLU		36	46.439	-8.689	6.522	1.00 24.53	В
								7.275	1.00 25.73	В
MOTA	1711	CA	GLU		36	45.332	-9.263			
MOTA	1712	CB	GLU	В	36	44.023	-8.519	6.958	1.00 26.62	В
MOTA	1713	CG	GLU	В	36	42.783	-9.095	7.636	1.00 28.26	В
MOTA	1714	CD	GLΰ	В	36	41.545	-8.232	7.442	1.00 31.08	В
ATOM	1715		GLU		36	41.420	-7.590	6.377	1.00 32.56	В
MOTA	1716		GLU		36	40.685	-8.206	8.349	1.00 32.83	В
MOTA	1717	С	GLU	В	36	45.238	-10.717	6.822	1.00 24.67	В
MOTA	1718	0	GLU	В	36	45.141	-10.992	5.626	1.00 23.91	В
ATOM	1719	N	ILE	В	37	45.282	-11.647	7.771	1.00 26.11	В
			ILE		37		-13.067	7.433	1.00 27.80	В
ATOM	1720	CA								
ATOM	1721	CB	ILE		37		-13.822	8.013	1.00 27.27	В
MOTA	1722	CG2	ILE	В	37	47.728	-13.174	7.516	1.00 27.41	В
ATOM	1723	CG1	ILE	В	37	46.440	-13.767	9.537	1.00 29.35	В
ATOM	1724		ILE		37		-14.509	10.175	1.00 30.27	В
								7.879	1.00 27.86	В
ATOM	1725	C	ILE		37		-13.750			
ATOM	1726	0	ILE	В	37		-14.674	7.221	1.00 28.29	В
ATOM	1727	N	VAL	В	38	43.348	-13.296	8.989	1.00 28.78	В
ATOM	1728	CA	VAL	В	38	42.097	-13.870	9.487	1.00 29.29	В
ATOM	1729	СВ	VAL		38		-14.751	10.741	1.00 30.18	В
								11.071	1.00 33.17	В
ATOM	1730		VAL		38		-15.452			
ATOM	1731	CG2	VAL	В	38		-15.764	10.520	1.00 31.09	В
MOTA	1732	С	VAL	В	38	41.161	-12.745	9.882	1.00 28.75	В
ATOM	1733	0	VAL	В	38	41.585	-11.758	10.480	1.00 29.70	В
	1734	N	ARG		39		-12.911	9.581	1.00 27.05	В
MOTA									1.00 25.46	В
ATOM	1735	CA	ARG		39		-11.890	9.892		
MOTA	1736	CB	ARG	В	39	38.627	-11.064	8.632	1.00 27.23	В
MOTA	1737	CG	ARG	В	39	37.544	-10.011	8.765	1.00 30.84	В
ATOM	1738	CD	ARG	В	39	37.111	-9.476	. 7.398	1.00 29.34	В
		NE	ARG		39	38.218		6.673	1.00 30.83	В
ATOM	1739								1.00 31.23	В
MOTA	1740	$^{\rm cz}$	ARG		39	38.116		5.459		
MOTA	1741	NH1	ARG	В	39	36.951	-8.333	4.823	1.00 31.08	В
ATOM	1742	NH2	ARG	В	39	39.178	-7.779	4.883	1.00 30.81	В
ATOM	1743	C	ARG	В	39	37.573	-12.476	10.381	1.00 25.41	В
ATOM	1744	ō	ARG		39		-13.587	9.996	1.00 25.06	В
										В
ATOM	1745	N	PHE		40		-11.742	11.252	1.00 23.72	
MOTA	1746	CA	PHE	В	40	35.569	-12.164	11.696	1.00 24.04	В
ATOM	1747	CB	PHE	В	40	35.498	-12.554	13.171	1.00 22.69	В
MOTA	1748	CG	PHE	В	40	34.133	-13.036	13.573	1.00 20.75	В
ATOM	1749		PHE		40		-14.370	13.413	1.00 21.07	В
							-12.135	14.003	1.00 21.00	В
MOTA	1750		PHE		40					
ATOM	1751	CE1	PHE	В	40		-14.800	13.670	1.00 20.86	В
MOTA	1752	CE2	PHE	В	40	31.858	-12.553	14.261	1.00 19.95	В
ATOM	1753	CZ	PHE	В	40	31.517	-13.890	14.092	1.00 19.78	В
ATOM	1754	c	PHE		40	34.662		11.474	1.00 24.27	В
						34.755		12.183	1.00 22.94	В
ATOM	1755	0	PHE		40					
MOTA	1756	N	ASP	В	41		-11.088	10.471	1.00 24.75	В
MOTA	1757	CA	ASP	В	41	32.857	-10.040	10.101	1.00 24.98	В
MOTA	1758	CB	ASP	В	41	32.863	-9.881	8.578	1.00 25.64	В
ATOM	1759	CG	ASF		41	32.162		8.116	1.00 27.70	В
						31.163		8.749	1.00 26.21	В
MOTA	1760		. ASE		41					
ATOM	1761		: ASF		41	32.607		7.102	1.00 30.42	В
ATOM	1762	C	ASE	В	41	31.477	-10.497	10.560	1.00 24.50	В
ATOM	1763	0	ASE	В	41	31.011	-11.558	10.151	1.00 24.95	В
ATOM	1764	N	SBF		42	30.822		11.404	1.00 24.16	В
					42		-10.096	11.882	1.00 26.13	В
MOTA	1765	CA	SEF						1.00 24.53	В
MOTA	1766	CB	SEF		42	29.013		12.972		
MOTA	1767	OG	SEF	B	42	28.932		12.497	1.00 23.39	В
ATOM	1768	C	SEF	B	42	28.497	-10.149	10.729	1.00 27.68	В
ATOM	1769	o	SEF		42	27.474	-10.833	10.818	1.00 27.31	В
			ASI		43	28.789		9.654	1.00 28.17	В
ATOM	1770	N							1.00 29.40	В
ATOM	1771	CA	ASI	י צ	43	27.924	-9.413	8.477	2.00 23.40	

MOTA	1772	СВ	ASP	В	43	28.332	-8.298	7.508	1.00 29.57	В
MOTA	1773		ASP		43	27.587	-7.006	7.766	1.00 32.71	В
MOTA	1774		ASP		43	26.999	-6.868	8.862	1.00 33.94	В
ATOM	1775		ASP		43	27.593	-6.120	6.881	1.00 33.98	B
ATOM	1776	C 0	ASP ASP		43 43	28.036 - 27.162 -		7.782 7.009	1.00 29.46 1.00 30.77	В
ATOM ATOM	1777 1778	N	VAL		44	29.123 -		8.068	1.00 27.98	В
ATOM	1779	CA	VAL		44	29.365 -		7.486	1.00 27.16	В
ATOM	1780	СВ	VAL		44	30.846		7.075	1.00 27.32	В
ATOM	1781	CG1	VAL	В	44	31.083 -	-14.323	6.488	1.00 24.09	В
MOTA	1782	CG2	VAL		44	31.218 -		6.073	1.00 24.66	В
MOTA	1783	С	VAL		44	28.990		8.490	1.00 28.43	В
ATOM	1784	0	VAL		44	28.558		8.108	1.00 29.45 1.00 28.05	B B
ATOM	1785	N	GLY GLY		45 45	29.177 - 28.794 -		9.774 10.780	1.00 28.67	В
ATOM ATOM	1786 1787	CA. C	GTA		45	29.758		11.125	1.00 28.25	В
ATOM	1788	ō	GLY		45	29.458		12.002	1.00 29.67	В
ATOM	1789	N	GLU		46	30.895		10.443	1.00 27.03	В
ATOM	1790	CA	GLU	В	46	31.873	-16.787	10.757	1.00 29.26	В
ATOM	1791	CB	GLU	В	46	31.571		10.000	1.00 32.16	В
ATOM	1792	CG	GLU		46	32.039		8.554	1.00 37.36	В
ATOM	1793	CD	GLU		46	31.752		7.885	1.00 41.59 1.00 43.30	B B
ATOM	1794		GLU		46 46	32.163 · 31.116 ·		8.433 6.810	1.00 43.54	В
ATOM	1795 1796	C C	GLU		46	33.272		10.413	1.00 29.29	В
ATOM ATOM	1797	ō	GLU		46	33.432		9.722	1.00 30.45	В
ATOM	1798	N	PHE		47	34.281		10.904	1.00 28.00	В
ATOM	1799	CA	PHE		47	35.670	-16.650	10.651	1.00 28.10	В
ATOM	1800	CB	PHE	В	47	36.594		11.566	1.00 28.74	В
MOTA	1801	CG	PHE		47	36.487		13.016	1.00 30.23	В
MOTA	1802		PHE		47	37.248		13.535 13.870	1.00 28.96 1.00 30.80	B B
ATOM	1803		PHE		47 47	35.636 37.166		14.888	1.00 30.50	В
ATOM ATOM	1804 1805		PHE		47	35.544		15.229	1.00 31.97	В
ATOM	1806	CZ	PHE		47	36.311		15.737	1.00 30.36	В
ATOM	1807	c	PHE		47	36.034		9.211	1.00 28.71	В
ATOM	1808	0	PHE		47	35.576	-17.937	8.640	1.00 28.03	В
ATOM	1809	N	ARG	В	48	36.872		8.637	1.00 27.96	В
MOTA	1810	CA	ARG		48	37.327		7.261	1.00 26.41	В
ATOM	1811	CB	ARG		48	36.513		6.326 6.108	1.00 26.57 1.00 26.19	B B
MOTA	1812	CG	ARG		48 48	35.068 34.971		5.352	1.00 24.98	В
MOTA MOTA	1813 1814	NE	ARG		48	33.579		5.146	1.00 26.01	В
ATOM	1815	CZ	ARG		48		-16.867	4.294	1.00 26.84	В
MOTA	1816		ARG		48		-15.857	3.554	1.00 26.92	В
ATOM	1817	NH2	ARC	В	48	31.492	-17.260	4.204	1.00 30.22	В
MOTA	1818	C	ARC	3 B	48		-15.861	7.140	1.00 26.95	В
MOTA	1819	0	ARG		48		-14.878	7.737	1.00 24.36	В
MOTA	1820	N	ALA		49		-16.647	6.373 6.143	1.00 24.93 1.00 26.58	B
ATOM	1821	CA CB	AL/ AL/		49 49		-16.349 -17.619	5.792	1.00 27.05	В
ATOM ATOM	1822 1823	C	AL		49		-15.397	4.956	1.00 26.47	В
MOTA	1824	ō	AL		49		-15.635	3.983	1.00 26.12	В
ATOM	1825	N	VAI		50		-14.302	5.044	1.00 27.06	В
ATOM	1826	CA	VAI		50		-13.357	3.936	1.00 26.50	В
MOTA	1827	CB		ьв	50		-11.876	4.439	1.00 27.14	В
ATOM	1828		VAI		50		-11.827	5.846 3.501	1.00 29.89 1.00 27.33	B B
MOTA	1829		VAJ	L B	50 50		-11.020 -13.742	3.037	1.00 26.58	В
MOTA MOTA	1830 1831	0		ĹΒ			-13.390	1.860	1.00 27.84	В
ATOM	1832	N		RB			-14.489	3.598	1.00 26.61	В
ATOM	1833	CA		RВ			-15.011	2.846	1.00 28.59	В
MOTA	1834	CB		RВ		46.295	-14.193	3.056	1.00 28.25	В
MOTA	1835		L TH				-14.464	4.356	1.00 28.56	В
MOTA	1836		2 TH				-12.699	2.899	1.00 27.40 1.00 29.29	B
MOTA	1837	C		R B			-16.435 -16.818	3.344 4.418	1.00 29.29	В
MOTA	1838	N O		R B U B			-17.217	2.575	1.00 30.64	В
MOTA MOTA	1839 1840	CA		U B			-18.596	2.959	1.00 31.32	В
ATOM	1841	CB		UΒ			-19.237	1.963	1.00 32.19	В
ATOM	1842	CG		UΒ		46.706	-19.724	0.624	1.00 36.90	В
ATOM	1843		1 LE				-20.306	-0.216	1.00 35.68	В
MOTA	1844		2 LE				-20.775	0.861	1.00 35.34	B
MOTA	1845	С	LE	UP	52	46.892	-18.724	4.359	1.00 31.57	В

		_				45 550	20 656	r 005	1 00 13 50	-
ATOM	1846	0	LEU I		2	46.570		5.097	1.00 31.50	В
ATOM	1847	N	LEU I		53	47.753		4.723	1.00 31.09	В
ATOM	1848	CA	LEU I	3 9	53	48.388	-17.815	6.029	1.00 30.93	В
ATOM	1849	CB	LEU I	8 5	53	49.160	-16.511	6.246	1.00 31.99	В
ATOM	1850	CG	TEO I	B 5	53	50.338	-16.532	7.221	1.00 35.20	В
ATOM	1851		LEU I		33	51.364	-17.559	6.763	1.00 35.92	В
			TEO I		53	50.975		7.284	1.00 34.96	В
ATOM	1852									В
MOTA	1853	C	TEO 1		53	47.377		7.160	1.00 29.90	
ATOM	1854	0	LEU 1	B 9	53	47.663	-18.709	8.138	1.00 30.68	В
ATOM	1855	N	GLY I	В 5	54	46.192	-17.430	7.015	1.00 28.63	В
MOTA	1856	CA	GLY 1	в 9	54	45.181	-17.537	8.057	1.00 29.75	В
ATOM	1857	C	GLY I		54	44.140		7.901	1.00 30.44	В
		o	GLY I		54	43.146		8.630	1.00 28.02	В
ATOM	1858								1.00 30.54	В
ATOM	1859	N	TEO :		55	44.364		6.964		
ATOM	1860	CA	LEU :	В !	55	43.417	-20.630	6.732	1.00 32.59	В
ATOM	1861	CB	TEO :	В!	55	43.765	-21.344	5.422	1.00 35.94	В
ATOM	1862	CG	LEU :	в 9	55	42.776	-22.383	4.889	1.00 38.88	В
ATOM	1863		LEU :		55	41.355	-21.831	4.927	1.00 38.23	В
	1864		LEU		55	43.173		3.467	1.00 39.03	В
ATOM									1.00 32.20	В
ATOM	1865	С	LEU :		55	43.330		7.892		
ATOM	1866	0	LEU :	В	55	42.235		8.291	1.00 33.32	В
MOTA	1867	N	PRO	в :	56	44.478	-22.058	8.447	1.00 31.03	В
MOTA	1868	CD	PRO	в :	56	45.862	-21.802	8.009	1.00 30.17	В
MOTA	1869	CA	PRO		56	44.451	-23.013	9.561	1.00 30.23	В
	1870	СВ	PRO		56	45.925		9.931	1.00 30.27	В
MOTA						46.609		8.610	1.00 28.92	В
MOTA	1871	CG	PRO		56					
MOTA	1872	C	PRO	В	56	43.613		10.740	1.00 31.42	В
ATOM	1873	0	PRO	В	56	42.730	-23.237	11.222	1.00 33.17	В
ATOM	1874	N	ALA	В	57	43.893	-21.305	11.196	1.00 30.04	В
ATOM	1875	CA	ALA		57	43.181	-20.719	12.322	1.00 28.60	В
	1876	СВ	ALA		57	43.818		12.697	1.00 26.81	В
ATOM								12.021	1.00 29.08	В
ATOM	1877	C	ALA		57 	41.695				
MOTA	1878	0	ALA		57		-20.737	12.887	1.00 28.22	В
MOTA	1879	N	ALA	В	58	41.385	-20.135	10.791	1.00 28.84	В
MOTA	1880	CA	ALA	В	58	40.002	-19.922	10.386	1.00 31.06	В
MOTA	1881	СВ	ALA		58	39.955	-19.426	8.947	1.00 29.79	В
		c	ALA		58		-21.199	10.529	1.00 32.38	В
ATOM	1882							11.170	1.00 31.57.	В
ATOM	1883	0	ALA		58		-21.197			
MOTA	1884	N	GLU	В	59		-22.285	9.929	1.00 33.50	B
ATOM	1885	CA	GLU	В	59	38.949	-23.565	9.993	1.00 33.91	В
MOTA	1886	CB	GLU	В	59	39.706	-24.622	9.195	1.00 35.67	В
MOTA	1887	CG	GLU		59	39.619	-24.457	7.696	1.00 39.73	В
ATOM	1888	CD	GLU		59		-25.583	6.957	1.00 43.58	В
			. GLU		59		-25.715	7.119	1.00 44.52	В
MOTA	1889							6.222	1.00 44.30	В
MOTA	1890	OE2			59		-26.337			
MOTA	1891	C	GLU	В	59		-24.063	11.425	1.00 33.56	В
MOTA	1892	0	GLU	В	59	37.708	-24.570	11.790	1.00 34.40	В
MOTA	1893	N	TYR	В	60	39.815	-23.923	12.233	1.00 31.99	В
ATOM	1894	CA	TYR	В	60	39.754	-24.369	13.611	1.00 31.01	В
ATOM	1895	CB	TYR		60		-24.202	14.292	1.00 31.13	В
			TYR		60		-24.548	15.750	1.00 30.99	В
MOTA	1896	CG								В
MOTA	1897	CD			60		-25.871	16.162	1.00 32.55	
ATOM	1898	CB:	LTYR	В	60		-26.192	17.508	1.00 35.39	В
MOTA	1899	CD	TYR	В	60	41.039	-23.550	16.716	1.00 32.67	В
ATOM	1900	CE	TYR	В	60	40.890	-23.853	18.064	1.00 35.14	В
ATOM	1901	CZ	TYR	В	60	40.756	-25.177	18.455	1.00 36.91	В
		OH	TYR		60		-25.483	19.791	1.00 40.06	В
ATOM	1902				60		-23.631	14.426	1.00 31.72	В
ATOM	1903	C	TYR							В
ATOM	1904	0	TYR		60		-24.258	15.050	1.00 31.72	
MOTA	1905	N	TRP	В	61	38.752	-22.303	14.428	1.00 30.37	В
ATOM	1906	CA	TRP	В	61	37.790	-21.525	15.194	1.00 31.57	В
MOTA	1907	CB	TRP	В	61	38.129	-20.024	15.140	1.00 32.14	В
ATOM	1908	CG	TRP		61	39,430	-19.666	15.824	1.00 33.73	В
			2 TRP		61		-18.648	15.429	1.00 35.16	В
MOTA	1909						-18.662	16.362	1.00 35.99	В
MOTA	1910		2 TRP		61					В
ATOM	1911		3 TRP		61		-17.719	14.378	1.00 38.30	
MOTA	1912		1 TRP		61		-20.236	16.949	1.00 33.63	В
MOTA	1913	NE	1 TRP	В	61	41.142	-19.642	17.278	1.00 33.97	В
MOTA	1914	CZ	2 TRP	В	61	42.512	-17.782	16.277	1.00 38.13	В
MOTA	1915		3 TRP		61	41.487	-16.836	14.293	1.00 39.26	В
ATOM	1916		2 TRP		61		-16.879	15.240	1.00 38.22	В
			TRP		61		-21.758	14.739	1.00 31.22	В
MOTA	1917						-21.758	15.559	1.00 29.98	В
MOTA	1918		TRP		61					
MOTA	1919	N	ASN	В	62	50.137	-21.955	13.440	1.00 31.63	В

MOTA	1920	CA	ASN E		34.781 -22.191	12.950	1.00 32.57	В
MOTA	1921	CB	ASN E	62	34.701 -22.021	11.434	1.00 30.37	· B
ATOM	1922	CG	ASN E	62	34.575 -20.574	11.025	1.00 29.69	В
ATOM	1923	OD1	ASN E	62	33.889 -19.794	11.680	1.00 29.42	В
ATOM	1924		ASN E		35.222 -20.209	9.926	1.00 31.50	В
					34.238 -23.561	13.339	1.00 32.87	В
ATOM	1925	C	ASN E					
MOTA	1926	0	ASN E		33.028 -23.789	13.292	1.00 34.70	В
MOTA	1927	N	SER E	63	35.128 -24.469	13.725	1.00 32.43	В
MOTA	1928	CA	SER E	63	34.705 -25.797	14.140	1.00 32.38	В
ATOM	1929	СВ	SER E		35.818 -26.819	13.879	1.00 32.20	В
		OG			36.905 -26.626	14.760	1.00 33.33	В
MOTA	1930		SER F					
ATOM	1931	С	SER E		34.348 -25.768	15.630	1.00 32.14	В
MOTA	1932	0	SER E	3 63	33.677 -26.667	16.138	1.00 32.86	В
MOTA	1933	N	GLN E	3 64	34.794 -24.724	16.325	1.00 31.10	В
MOTA	1934	CA	GLN E	3 64	34.513 -24.569	17.752	1.00 30.99	В
ATOM	1935	CB	GLN E		35.661 -23.837	18.446	1.00 32.54	В
			GIN I		36.988 -24.557	18.383	1.00 34.49	В
MOTA	1936	CG						
MOTA	1937	æ	GLN F		36.870 -25.998	18.810	1.00 38.20	В
MOTA	1938	OE1	GLN F	3 64	36.629 -26.884	17.984	1.00 40.82	В
ATOM	1939	NE2	GLN I	B 64	37.022 -26.245	20.108	1.00 38.34	В
ATOM	1940	C	GLN I	3 64	33.226 -23.775	17.944	1.00 29.88	В
ATOM	1941	ō	GLN I		33.252 -22.549	18.064	1.00 29.28	В
					32.101 -24.476	17.979	1.00 28.74	В
ATOM	1942	N	LYS I					
ATOM	1943	CA	LYS I		30.815 -23.812	18.123	1.00 29.18	В
MOTA	1944	CB	LYS I	B 65	29.688 -24.851	18.132	1.00 30.63	В
ATOM	1945	CG	LYS 1	B 65	29.575 -25.612	16.812	1.00 32.20	В
ATOM	1946	œ	LYS I	B 65	29.371 -24.654	15.629	1.00 34.44	В
ATOM	1947	CE	LYS		29.688 -25.327		1.00 37.24	В
					29.430 -24.427		1.00 37.89	В
MOTA	1948	NZ	LYS					
ATOM	1949	С	LYS :		30.745 -22.919		1.00 28.19	В
ATOM	1950	0	LYS	B 65	30.075 -21.891	19.333	1.00 28.16	В
ATOM	1951	N	ASP I	B 66	31.440 -23.304	20.417	1.00 27.58	В
ATOM	1952	CA	ASP :	B 66	31.460 -22.504	21.636	1.00 27.41	В
	1953	СВ	ASP		32.283 -23.208		1.00 28.45	В
MOTA							1.00 32.24	В
MOTA	1954	CG	ASP		33.559 -23.847			
MOTA	1955	OD1	ASP :		33.478 -24.591		1.00 33.17	В
ATOM	1956	OD2	ASP :	B 66	34.642 -23.623	22.765	1.00 33.25	В
ATOM	1957	C	ASP :	B 66	32.050 -21.131	21.316	1.00 26.63	В
ATOM	1958	o	ASP :		31.468 -20.102	21.662	1.00 24.32	В
		N	ILE		33.198 -21.116		1.00 26.12	В
ATOM	1959						1.00 26.42	В
ATOM	1960	CA	ILE :		33.840 -19.855			
MOTA	1961	CB	ILE :	B 67	35.206 -20.088		1.00 28.29	В
ATOM	1962	CG2	ILE :	B 67	35.859 -18.753	19.290	1.00 28.54	В
ATOM	1963	CG1	ILE	B 67	36.094 -20.925	20.535	1.00 28.25	В
ATOM	1964		ILE		36.319 -20.321	21.906	1.00 32.66	В
ATOM	1965	C	ILE		32.968 -19.061		1.00 26.36	В
					32.747 -17.869		1.00 25.33	В
MOTA	1966	0	ILE					В
MOTA	1967	N	LEU		32.472 -19.730		1.00 26.11	
MOTA	1968	CA	LEU	B 68	31.617 -19.086		1.00 26.66	В
MOTA	1969	CB	LEU	B 68	31.132 -20.102	16.235	1.00 27.61	В
ATOM	1970	CG	LEU	B 68	31.807 -20.171	14.872	1.00 30.12	В
ATOM	1971		LEU	B 68	31.081 -21.216	14.031	1.00 33.09	В
	1972		LEU		31.766 -18.812		1.00 30.01	В
MOTA							1.00 26.81	В
MOTA	1973	С	LEO		30.394 -18.415			
ATOM	1974	0	LEU		30.067 -17.280		1.00 26.19	В
MOTA	1975	N	GLU	B 69	29.706 -19.135		1.00 28.87	В
ATOM	1976	CA	GLU	B 69	28.509 -18.614	19.404	1.00 31.55	В
MOTA	1977	CB	GLU	B 69	27.945 -19.654	20.382	1.00 35.75	В
MOTA	1978	CG	GLU		27.304 -20.862		1.00 43.71	В
		æ	GLU		26.883 -21.954		1.00 47.92	В
MOTA	1979						1.00 49.27	В
MOTA	1980		GLU		27.756 -22.454			
MOTA	1981	OE2	GLU	B 69	25.683 -22.316		1.00 50.44	В
ATOM	1982	C	GLU	B 69	28.773 -17.29		1.00 29.82	В
ATOM	1983	0	GLU	B 69	27.986 -16.356	20.027	1.00 27.91	В
ATOM	1984	N	ARG		29.886 -17.226		1.00 29.32	В
		CA	ARG		30.239 -16.01		1.00 28.97	В
ATOM	1985						1.00 28.94	В
ATOM	1986	CB	ARG		31.347 -16.31		1.00 30.55	В
ATOM	1987	CG	ARG		30.982 -17.34			
ATOM	1988	CD	ARG		32.251 -17.81		1.00 32.35	. В
MOTA	1989	NE	ARG	B 70	32.040 -19.03		1.00 34.83	В
ATOM	1990	CZ	ARG	B 70	32.946 -19.99	7 25.232	1.00 34.98	В
ATOM	1991		1 ARG		34.131 -19.87		1.00 35.03	В
			2 ARG		32.662 -21.08		1.00 39.48	В
ATOM	1992						1.00 26.77	В
MOTA	1993	C	ARG	B 70	30.691 -14.88		#0.77	_

ATOM	1994	0	ARG	В	70	30.412	-13.725	20.951	1.00 26.95	В
ATOM	1995	N	LYS		71	31.395		19.608	1.00 25.97	В
ATOM	1996	CA	LYS	В	71	31.885	-14.236	18.670	1.00 25.98	В
MOTA	1997	CB	Lys	В	71	32.830	-14.877	17.652	1.00 27.62	В
ATOM	1998	CG	LYS	В	71	33.728		16.924	1.00 29.24	В
MOTA	1999	CD	Lys		71	34.628		17.909	1.00 32.14	В
MOTA	2000	CE	LYS		71	35.430		17.236	1.00 33.13	B B
ATOM	2001	NZ	LYS		71	36.093		18.245	1.00 34.18 1.00 25.22	В
ATOM	2002	C	LYS		71	30.710 30.719		17.952 17.671	1.00 25.22	В
ATOM	2003	0	LYS		71	29.701		17.657	1.00 25.08	В
ATOM	2004	N	ARG		72 72	28.500		16.989	1.00 26.32	В
MOTA MOTA	2005 2006	CA CB	ARG		72	27.628		16.561	1.00 2B.02	В
ATOM	2007	CG	ARG		72	28.116		15.340	1.00 28.10	В
ATOM	2008	CD	ARG		72	27.225		15.083	1.00 32.02	В
ATOM	2009	NE	ARG		72	27.451		13.766	1.00 36.46	В
ATOM	2010	CZ	ARG	В	72	27.014	-18.779	13.389	1.00 38.62	В
ATOM	2011		ARG	В	72	26.324	-19.538	14.238	1.00 37.88	В
ATOM	2012	NH2	ARG	В	72		-19.212	12.163	1.00 38.55	В
ATOM	2013	C	ARG	В	72		-13.017	17.898	1.00 24.31	В
ATOM	2014	0	ARG		72		-12.326	17.439	1.00 24.84	В
MOTA	2015	N	ALA		73		-13.028	19.189	1.00 26.18	B B
MOTA	2016	CA	ALA		73		-12.185	20.140	1.00 28.18 1.00 28.97	В
MOTA	2017	CB	ALA		73		-12.974	20.472	1.00 28.97	В
MOTA	2018	C	ALA		73	28.056	-10.916 -9.977	21.066	1.00 30.50	В
MOTA	2019	0	ALA ALA		73 74		-10.882	20.070	1.00 29.65	В
ATOM	2020	N CA	ALA		74	30.170	-9.732	20.347	1.00 30.77	В
MOTA MOTA	2021 2022	CB	ALA		74	31.558	-9.966	19.764	1.00 30.77	В
ATOM	2022	c	ALA		74	29.594	-8.414	19.827	1.00 31.78	В
ATOM	2024	ō	ALA		74	29.789	-7.359	20.438	1.00 32.74	В
ATOM	2025	N	VAL		75	28.886	-8.465	18.704	1.00 31.60	В
ATOM	2026	CA	VAL	В	75	28.308	-7.248	18.145	1.00 32.38	В
ATOM	2027	CB	VAL	В	75	27.397	-7.539	16.929	1.00 30.51	В
MOTA	2028	CG1	VAI	В	75	27.291	-6.295	16.062	1.00 31.44	В
MOTA	2029	CG2	VAI		75	27.931	-8.696	16.137	1.00 33.08	В
MOTA	2030	С	VAI		75	27.465	-6.529	19.201	1.00 33.07	B
MOTA	2031	0	VAI		75	27.402	-5.302	19.218	1.00 33.54 1.00 34.70	В
MOTA	2032	N	ASI		76	26.811	-7.302	20.065 21.130	1.00 36.27	В
ATOM	2033	CA	ASI		76 76	25.971 24.780	-6.748 -7.670	21.420	1.00 38.57	В
ATOM	2034	CB	ASI ASI		76	23.889	-7.881	20.215	1.00 41.48	В
MOTA MOTA	2035 2036		ASI		76	23.335	-6.887	19.694	1.00 43.46	В
ATOM	2037		ASI		76	23.739	-9.048	19.792	1.00 43.76	В
ATOM	2038	C	ASI		76	26.780	-6.600	22.411	1.00 35.56	В
ATOM	2039	ō	ASI		76	26.731	-5.569	23.081	1.00 34.13	В
ATOM	2040	N	ARC	3 В	77	27.508	-7.661	22.744	1.00 35.22	В
MOTA	2041	CA	AR	3 B	77	28.343	-7.708	23.937	1.00 34.49	В
ATOM	2042	CB		3 B	77	29.071	-9.052	23.991	1.00 37.16	В
MOTA	2043	CG		3 B	77	29.841	-9.328	25.271	1.00 40.90	B B
MOTA	2044	CD.		3 B	77		-10.553	25.102 24.665	1.00 43.79 1.00 48.65	В
MOTA	2045	NE		3 B	77		-11.743 -12.385	25.406	1.00 51.36	В
MOTA	2046	CZ	AR L AR	3 B	77 77		-11.949	26.626	1.00 52.34	В
ATOM ATOM	2047 2048		2 AR				-13.470	24.935	1.00 50.76	В
ATOM	2049	C		GB		29.362		23.927	1.00 32.18	В
ATOM	2050	ō		GВ		29.499		24.896	1.00 32.49	В
ATOM	2051	N	VA	LВ	78	30.073	-6.442	22.818	1.00 30.66	В
MOTA	2052	CA	VA	L B	78	31.086		22.707	.1.00 29.00	В
MOTA	2053	CB		L B		32.276		21.867	1.00 27.82	В
MOTA	2054		1 VA			33.327		21.740	1.00 25.08	B B
ATOM	2055		2 VA			32.870			1.00 23.27 1.00 29.33	В
MOTA	2056			L B		30.594			1.00 29.83	B
MOTA	2057			T E		30.435			1.00 28.42	В
MOTA	2058			S E		30.354 29.927			1.00 29.14	В
MOTA	2059 2060			SE		28.724				В
ATOM ATOM	2061			SE		28.883				В
MOTA	2062			SE		29.675				В
MOTA	2063			S		31.052				В
ATOM	2064			eg E		27.52				В
ATOM	2065			lG I		26.34				В
MOTA	2066			ig i		25.079				B
MOTA	2067	7 CG	AF	ig i	80	24.61	2 -2.973	19.474	1.00 35.65	В

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MOTA	2068	æ	ARG	В	80	23.120	-3.273	19.387	1.00 36.01	В
ATOM	2069	NE	ARG	В	80	22.649	-3.243	18.005	1.00 35.49	В
MOTA	2070	CZ	ARG	В	80	22.913	-4.188	17.108	1.00 37.80	В
ATOM	2071		ARG	В	80	23.640	-5.242	17.449	1.00 40.57	В
ATOM	2072		ARG		80	22.467	-4.075	15.864	1.00 38.86	В
					80	26.507	-1.552	22.524	1.00 31.24	В
ATOM	2073	C	ARG							В
MOTA	2074	0	ARG		80	25.975	-0.525	22.944	1.00 32.07	
ATOM	2075	N	HIS	В	81	27.257	-2.337	23.283	1.00 31.40	В
ATOM	2076	CA	HIS	В	81	27.492	-2.028	24.683	1.00 32.20	В
ATOM	2077	CB	HIS	В	81	28.220	-3.185	25.366	1.00 33.00	В
ATOM	2078	CG	HIS		81	28.595	-2.899	26.787	1.00 37.24	В
ATOM	2079		HIS		81	29.764	-2.490	27.335	1.00 38.05	В
			HIS		81	27.692	-2.981	27.826	1.00 39.11	В
ATOM	2080							28.952	1.00 40.49	В
ATOM	2081		HIS		81	28.290	-2.635			
MOTA	2082		HIS		81	29.548	-2.332	28.682	1.00 39.16	В
MOTA	2083	C	HIS	В	81	28.326	-0.762	24.831	1.00 30.87	В
ATOM	2084	0	HIS	В	81	27.906	0.206	25.470	1.00 31.38	В
MOTA	2085	N	ASN	В	82	29.511	-0.770	24.233	1.00 29.77	В
ATOM	2086	CA	ASN	В	82	30.403	0.375	24.332	1.00 28.02	B
MOTA	2087	CB	ASN		82	31.755	0.056	23.683	1.00 26.64	В
			ASN		82	32.470	-1.092	24.373	1.00 25.02	В
ATOM	2088	CG							1.00 24.06	В
MOTA	2089		ASN		82	32.305	-1.305	25.572		
ATOM	2090	ND2	asn	В	82	33.278	-1.829	23.619	1.00 26.38	В
MOTA	2091	C	asn	В	82	29.819	1.648	23.741	1.00 26.04	В
MOTA	2092	0	ASN	В	82	30.163	2.747	24.174	1.00 25.71	В
ATOM	2093	N	TYR	В	83	28.930	1.512	22.765	1.00 25.90	В
ATOM	2094	CA	TYR		83	28.324	2.693	22.156	1.00 25.91	В
	2095	СВ	TYR		83	27.462	2.297	20.946	1.00 25.69	В
MOTA						27.102	3.462	20.056	1.00 25.95	В
MOTA	2096	CG	TYR		83					В
MOTA	2097		TYR		83	26.022	4.294	20.353	1.00 27.11	
MOTA	2098	CE1	TYR	В	83	25.712	5.403	19.545	1.00 25.98	В
MOTA	2099	CD2	TYR	В	83	27.865	3.759	18.933	1.00 27.72	В
MOTA	2100	CE2	TYR	В	83	27.567	4.862	18.121	1.00 28.05	В
MOTA	2101	CZ	TYR		83	26.493	5.680	18.434	1.00 27.73	В
ATOM	2102	OH	TYR		83	26.225	6.781	17.645	1.00 27.55	В
			TYR		83	27.485	3.458	23.181	1.00 25.87	В
ATOM	2103	C						23.070	1.00 26.05	В
ATOM	2104	0	TYR		83	27.315	4.673			
MOTA	2105	N	GLN	В	84	26.975	2.750	24.186	1.00 28.25	В
MOTA	2106	CA	GFN	В	84	26.159	3.375	25.229	1.00 30.44	В
MOTA	2107	CB	GLN	В	84	25.467	2.310	26.093	1.00 34.30	В
ATOM	2108	CG	GLN	В	84	24.595	1.343	25.301	1.00 40.52	В
ATOM	2109	CD	GLN		84	23.515	2.047	24.496	1.00 43.21	В
ATOM	2110		GLN		84	23.023	1.516	23.499	1.00 46.12	В
			GLN		84	23.133	3.244	24.932	1.00 45.41	В
ATOM	2111						4.254	26.111	1.00 29.01	В
MOTA	2112	C	GLN		84	27.030				В
MOTA	2113	0	GLN		84	26.633	5.353	26.494	1.00 27.82	
ATOM	2114	N	LEU	В	85	28.219	3.757	26.436	1.00 28.32	В
ATOM	2115	CA	LEU	В	85	29.150	4.505	27.263	1.00 28.76	В
MOTA	2116	CB	LEU	В	85	30.355	3.631	27.631	1.00 28.92	В
ATOM	2117	CG	LEU	В	85	30.065	2,226	28.184	1.00 30.98	В
ATOM	2118		LEU		85	31.343	1.631	28.758	1.00 30.59	В
			LEU		85	29.006	2.291	29.265	1.00 31.87	В
MOTA	2119						5.719	26.461	1.00 29.95	В
MOTA	2120	C	LEU		85	29.609			1.00 30.93	В
ATOM	2121	0	LEU		85	29.836	6.798	27.010		
MOTA	2122	N	GLU		86	29.724	5.529	25.150	1.00 30.31	В
MOTA	2123	CA	GLU	В	86	30.160	6.577	24.245	1.00 31.41	В
MOTA	2124	CB	· GLU	В	86	30.426	5.981	22.861	1.00 32.60	В
MOTA	2125	CG	GLU	в	86	31.741	6.420	22.236	1.00 39.25	В
ATOM	2126	CD	GLU			32.962	5.854	22.953	1.00 41.02	В
ATOM	2127		1 GLU			33.379	4.714	22.636	1.00 40.75	В
						33.497	6.553	23.843	1.00 41.96	В
MOTA	2128		2 GLU						1.00 32.44	В
MOTA	2129	С	GLU			29.113	7.684	24.146		
MOTA	2130	0	GLU	JВ	86	29.454	8.865	24.109	1.00 30.73	В
MOTA	2131	N	LEU	JВ	87	27.838	7.303	24.103	1.00 33.77	В
MOTA	2132	CA	LEU	J B	87	26.755	8.282	24.015	1.00 34.65	В
ATOM	2133	СВ	LEU			25.398	7.583	23.899	1.00 34.69	В
ATOM	2134	CG				24.916	7.169	22.508	1.00 36.86	В
	2135		1 LET			23.655		22.642	1.00 35.43	В
MOTA						24.645		21.660	1.00 35.76	В
MOTA	2136		2 LET						1.00 35.76	В
MOTA	2137		LEI			26.740	_	25.231		
MOTA	2138		LE			26.250		25.164	1.00 34.29	В
MOTA	2139	N	AR	3 B	88	27.280		26.343		В
MOTA	2140	CA	AR	3 B	88	27.317	9.493	27.573		В
ATOM	2141	CB		3 E		27.173	8.575	28.791	1.00 39.79	В

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MOTA	2142	CG	ARG	В	88	25.827	7.878	28.908	1.00 45.19	В
MOTA	2143	CD	ARG	В	88	25.704	7.173	30.253	1.00 49.04	В
ATOM	2144	NB	ARG	В	88	26.657	6.074	30.388	1.00 54.57	В
	2145	CZ	ARG		88	27.101	5.603	31.552	1.00 55.76	В
ATOM									1.00 55.56	В
ATOM	2146		ARG		88	26.683	6.137	32.694		
ATOM	2147	NH2	ARG	В	88	27.963	4.595	31.574	1.00 56.11	В
MOTA	2148	C	ARG	В	88	28.601	10.299	27.714	1.00 36.93	В
ATOM	2149	0	ARG	R	88	28.702	11.160	28.589	1.00 37.24	В
							10.035	26.842	1.00 35.19	В
ATOM	2150	N	THR		89	29.571				
MOTA	2151	CA	THR	В	89	30.860	10.712	26.914	1.00 31.71	В
ATOM	2152	CB	THR	В	89	31.916	9.767	27.529	1.00 31.61	В
ATOM	2153	OG1	THR	В	89	31.980	8.554	26.762	1.00 29.72	В
ATOM	2154		THR		89	31.557	9.436	28.963	1.00 25.87	В
							11.254	25.600	1.00 31.31	В
ATOM	2155	C	THR		89	31.420				
MOTA	2156	0	THR	В	89	31.214	12.415	25.249	1.00 32.41	В
ATOM	2157	N	THR	В	90	32.139	10.403	24.880	1.00 30.72	В
MOTA	2158	CA	THR	В	90	32.766	10.786	23.623	1.00 30.43	В
ATOM	2159	СВ	THR		90	33.368	9.558	22.925	1.00 30.54	В
							8.919	23.808	1.00 33.70	В
ATOM	2160	OG1			90	34.297				
MOTA	2161	CG2	THR	В	90	34.099	9.970	21.666	1.00 31.65	В
MOTA	2162	С	THR	В	90	31.874	11.512	22.625	1.00 30.61	, В
ATOM	2163	0	THR	В	90	32.267	12.543	22.070	1.00 30.24	В
	2164	N	PEA		91	30.683	10.977	22.385	1.00 30.30	В
MOTA								21,425	1.00 31.93	В
MOTA	2165	ÇA	LEU		91	29.767	11.581			
MOTA	2166	CB	LEU	В	91	28.709	10.554	21.007	1.00 32.55	В
ATOM	2167	ÇG	LEU	В	91	29.268	9.315	20.292	1.00 33.01	В
MOTA	2168		LEU	R	91	28.201	8.233	20.205	1.00 33.73	В
			LEU		91	29.761	9.700	18.902	1.00 31.26	В
MOTA	2169								1.00 32.38	В
MOTA	2170	С	LEU		91	29.096	12.872	21.907		
MOTA	2171	0	LEU	В	91	28.402	13.534	21.139	1.00 32.08	В
MOTA	2172	N	GLN	В	92	29.303	13.229	23.173	1.00 32.44	В
ATOM	2173	CA	GLN	В	92	28.725	14.454	23.713	1.00 34.54	В
			GLN		92	28.138	14.217	25.110	1.00 38.48	В
ATOM	2174	CB							1.00 44.66	В
MOTA	2175	CG	GLN		92	26.836	13.419	25.121		
ATOM	2176	CD	GLN	В	92	26.233	13.291	26.516	1.00 49.27	В
ATOM	2177	OE1	GLN	В	92	25.239	12.588	26.712	1.00 51.65	В
ATOM	2178	NE2			92	26.832	13.975	27.491	1.00 49.93	В
					92	29.779	15.557	23.777	1.00 32.86	' В
MOTA	2179	C	GLN							В
MOTA	2180	0	GLN		92	29.457	16.721	24.019	1.00 32.19	
ATOM	2181	N	ARG	В	93	31.038	15.187	23.555	1.00 31.53	В
MOTA	2182	CA	ARG	В	93	32.132	16.157	23.576	1.00 29.87	В
ATOM	2183	СВ	ARG	R	93	33.477	15.472	23.302	1.00 28.14	В
			ARG		93	34.681	16.433	23.217	1.00 23.56	В
ATOM	2184	CG						22.925	1.00 22.53	В
MOTA	2185	æ	ARG		93	35.953	15.656			
ATOM	2186	NE	ARG	₿	93	37.128	16.486	22.662	1.00 19.19	В
ATOM	2187	cz	ARG	В	93	37.769	17.205	23.581	1.00 18.66	В
ATOM	2188	NH1	ARG	В	93	37.352	17.214	24.843	1.00 17.45	В
ATOM	2189	NH2			93	38.847	17.898	23.242	1.00 16.56	В
						31.921	17.245	22.535	1.00 29.02	В
MOTA	2190	C	ARG		93					В
MOTA	2191	0	ARG	В	93	31.75 5	16.965	21.349	1.00 29.55	
MOTA	2192	N	ARG	В	94	31.933	18.490	22.987	1.00 28.71	В
ATOM	2193	CA	ARG	В	94	31.767	19.613	22.087	1.00 29.63	В
ATOM	2194	CB	ARG		94	30.299	20.046	22.041	1.00 32.44	В
		CG	ARG		94	29.506	19.196	21.060	1.00 37.10	В
MOTA	2195						19.414	21.124	1.00 39.80	В
ATOM	2196	CD	ARG		94	28.016				
ATOM	2197	NE	ARG	В	94	27.350	18.742	20.008	1.00 44.04	В
MOTA	2198	CZ	ARG	В	94	27.372	17.428	19.791	1.00 44.11	В
ATOM	2199	NH	L ARG	В	94	28.026	16.625	20.617	1.00 45.60	В
	2200		2 ARG		94	26.747	16.916	18.739	1.00 44.45	В
MOTA								. 22.498	1.00 28.84	В
ATOM	2201	C	ARG		94	32.656				
MOTA	2202	0	ARG	В	94	32.464	21.363	23.550	1.00 29.13	В
MOTA	2203	N	VAL	В	95	33.650	21.038	21.663	1.00 27.49	В
ATOM	2204	CA			95	34.592	22.117	21.916	1.00 26.47	В
ATOM	2205	CB	VAL		95	36.047	21.605	21.890	1.00 25.65	В
						37.004	22.734	22.260	1.00 22.82	В
MOTA	2206		1 VAI		95					В
MOTA	2207	CG:	2 VAI		95	36.202	20.423	22.849	1.00 26.01	
ATOM	2208	C	VAI	В	95	34.415	23.180	20.840	1.00 27.00	В
MOTA	2209	0	VAI	В	95	34.721	22.945	19.665	1.00 27.00	В
ATOM	2210		GL			33.912		21.253	1.00 26.94	В
ATOM	2211					33.673				В
										В
MOTA	2212					33.072				
MOTA	2213	CG	GL	JB	96	31.736				В
ATOM	2214	CD	GLI	B	96	31.211	27.582			В
MOTA	2215		1 GL			30.121	27.477	23.144	1.00 42.85	В

MOTA	2216	OE2	GLU B	96	31.891	28.634	22.526	1.00 40.11	В
ATOM	2217	C	GLU B	96	34.960	25.916	19.689	1.00 25.02	В
ATOM	2218	0	GLU B	96	35.999	26.022	20.338	1.00 24.73	В
ATOM	2219		PRO B	97	34.900	26.204	18.383	1.00 24.54	В
MOTA	2220		PRO B	97	33.744	26.011	17.493	1.00 22.89	В
ATOM	2221		PRO B	97	36.069	26.655	17.626	1.00 23.87	В
ATOM	2222		PRO B	97	35.580	26.633	16.175	1.00 22.81	В
	2223		PRO B	97	34.411	25.663	16.202	1.00 25.55	В
ATOM							18.021	1.00 23.80	В
ATOM	2224		PRO B	97	36.498	28.061			В
MOTA	2225		PRO B	97	35.665	28.905	18.353	1.00 24.40	
MOTA	2226		THR B	98	37.799	28.307	17.990	1.00 22.02	В
MOTA	2227	CA	THR B	98	38.306	29.634	18.266	1.00 24.00	В
ATOM	2228	CB	THR B	98	39.569	29.592	19.150	1.00 27.31	В
ATOM	2229	OG1	THR B	98	40.626	28.929	18.449	1.00 35.69	В
ATOM	2230	CG2	THR B	98	39.282	28.839	20.439	1.00 26.76	В
ATOM	2231	C	THR B	98	38.631	30.143	16.860	1.00 22.38	В
ATOM	2232		THR B		39.376	29.504	16.116	1.00 19.48	В
MOTA	2233		VAL B		38.041	31.274	16.487	1.00 21.55	В
ATOM	2234		VAL B		38.242	31.824	15.152	1.00 21.20	В
			VAL B		36.871	32.153	14.509	1.00 21.09	В
ATOM	2235		VAL B			32.541	13.050	1.00 19.62	В
MOTA	2236				37.043			1.00 18.29	В
ATOM	2237		VAL B		35.950	30.944	14.625		В
ATOM	2238		VAL B		39.140	33.059	15.167	1.00 21.59	
ATOM	2239	0	VAL B		38.970	33.962	15.982	1.00 21.57	В
ATOM	2240		THR B		40.099	33.084	14.252	1.00 22.65	В
MOTA	2241	CA	THR B	100	41.056	34.179	14.168	1.00 24.95	В
MOTA	2242	CB	THR B	100	42.399	33.770	14.820	1.00 26.31	В
MOTA	2243	OG1	THR B	100	42.162	33.321	16.160	1.00 30.10	В
MOTA	2244	CG2	THR B	100	43.359	34.942	14.854	1.00 29.07	В
ATOM	2245	С	THR B	100	41.329	34.556	12.717	1.00 24.61	В
ATOM	2246	0	THR B		41.514	33.689	11.869	1.00 23.89	В
ATOM	2247	N	ILE B		41.363	35.852	12.435	1.00 26.18	В
	2248	CA	ILE B		41.638	36.315	11.080	1.00 29.32	В
MOTA					40.572	37.327	10.582	1.00 29.37	В
MOTA	2249	CB	ILE B				9.231	1.00 29.49	В
ATOM	2250		ILE B		40.986	37.885		1.00 30.11	В
ATOM	2251		IPE B		39.198	36.664	10.492		
ATOM	2252		IFE B		38.110	37.605	10.002	1.00 29.81	В
ATOM	2253	С	ILE B		42.988	37.015	11.040	1.00 31.04	В
ATOM	2254	0	ILE B	101	43.270	37.868	11.877	1.00 31.24	В
MOTA	2255	N	SER E	102	43.820	36.664	10.066	1.00 34.47	В
MOTA	2256	CA	SER E	102	45.124	37.303	9.940	1.00 39.17	В
ATOM	2257	CB	SER E	102	46.143	36.617	10.844	1.00 37.33	В
MOTA	2258	OG	SER E	102	46.326	35,265	10.462	1.00 41.93	В
ATOM	2259	С	SER E	102	45.632	37.289	8.501	1.00 42.45	В
ATOM	2260	0	SER E		45.641	36.248	7.845	1.00 42.45	В
MOTA	2261	N	PRO E		46.052	38.455	7.988	1.00 45.38	В
ATOM	2262	CD	PRO E		45.938	39.793	8.596	1.00 45.47	В
MOTA	2263	CA	PRO E		46.564	38.545	6.617	1.00 48.91	В
		CB	PRO E		46.446	40.032	6.312	1.00 47.74	В
MOTA	2264		PRO E		46.739	40.652	7.642		В
MOTA	2265	CG	PRO E		48.010	38.042	6.545	1.00 51.96	В
ATOM	2266	C				37.957	7.568	1.00 52.51	В
ATOM	2267	0	PRO E		48.688			1.00 55.84	В
MOTA	2268	N	SER E		48.475	37.699	5.346		В
MOTA	2269	CA	SER E		49.843	37.209	5.177	1.00 60.00	
ATOM	2270	CB	SER I		50.018	36.578	3.791	1.00 59.60	В
MOTA	2271	OG	SER I		49.778	37.520	2.759	1.00 59.05	В
MOTA	2272	C	SER I		50.842	38.353	5.368	1.00 63.75	В
MOTA	2273	0	SER I	3 104	50.853	39.325	4.605	1.00 64.64	В
MOTA	2274	N	ARG I	3 105	51.677	38.228	6.398	1.00 66.99	В
ATOM	2275	CA	ARG I	3 105	52.674	39.242	6.736	1.00 69.17	В
ATOM	2276	CB	ARG I	3 105	53.631	38.700	7.808	1.00 70.33	В
ATOM	2277	CG	ARG I	3 105	54.672	37.690	7.318	1.00 72.24	В
ATOM	2278	CD	ARG I		54.073	36.586	6.449	1.00 73.51	В
ATOM	2279	NE		B 105	52.981	35.859	7.095	1.00 75.02	В
ATOM	2280	CZ		B 105	53.120	35.051	8.142	1.00 76.07	В
			ARG		54.314	34.852	8.684	1.00 77.38	В
MOTA	2281				52.059	34.431	8.644	1.00 76.05	В
MOTA	2282		ARG I		53.464	39.720	5.523	1.00 70.38	В
ATOM	2283	C		B 105			4.923	1.00 70.36	В
MOTA	2284	0		B 105	53.134	40.746		1.00 /1.36	В
MOTA	2285	N		B 113	46.629	40.478	-1.867		В
ATOM	2286	CA.		B 113	46.963	40.039	-0.515	1.00 48.42	В
MOTA	2287	CB		B 113	46.726	41.181	0.477	1.00 51.23	В
MOTA	2288	CG		B 113	47.268	40.875	1.863	1.00 53.89	
MOTA	2289	OD1	ASN	B 113	48.429	40.498	2.019	1.00 55.14	В

ATOM	2290	ND2	ASN B :	113	46.428	41.048	2.880	1.00 55.30	B
MOTA	2291	C	ASN B	113	46.143	38.808	-0.118	1.00 45.78	В
MOTA	2292	0	ASN B.	113	45.155	38.471	-0.774	1.00 44.99	В
MOTA	2293	N	LEU B	114	46.550	38.146	0.961	1.00 42.27	В
ATOM	2294	CA	LEU B		45.862	36.944	1.415	1.00 38.77	В
ATOM	2295	СВ	LEU B		46.770	35.739	1.182	1.00 39.10	В
ATOM	2296	CG	LEU B		46.238	34.330	1.421	1.00 40.81	В
ATOM	2297		LEU B		45.097	34.023	0.459	1.00 41.59	В
			LEU B		47.379	33.341	1.222	1.00 41.03	В
ATOM	2298					36.986	2.883	1.00 36.39	В
ATOM	2299	C	LEU B		45.424			1.00 35.98	В
MOTA	2300	0	LEU B		46.237	37.204	3.783		
ATOM	2301	И	LEU B		44.130	36.777	3.112	1.00 31.79	В
MOTA	2302	CA	LEU B		43.576	36.766	4.460	1.00 28.77	В
ATOM	2303	CB	LEU B	115	42.231	37.496	4.493	1.00 29.52	В
ATOM	2304	CG	LEU B	115	42.156	38.843	5.218	1.00 30.12	В
ATOM	2305	CD1	LEU B	115	43.281	39.751	4.764	1.00 30.28	В
ATOM	2306	CD2	LEU B	115	40.799	39.479	4.951	1.00 28.39	В
ATOM	2307	C	LEU B	115	43.374	35.323	4.896	1.00 27.23	В
ATOM	2308	0	LEU B		42.815	34.513	4.154	1.00 25.72	В
ATOM	2309	N	VAL B		43.825	35.002	6.103	1.00 24.13	В
		CA	VAL B		43.695	33.651	6.618	1.00 20.76	В
ATOM	2310		VAL B		45.078	33.098	7.078	1.00 20.02	В
ATOM	2311	CB	VAL B		44.915	31.757	7.777	1.00 17.46	В
ATOM	2312						5.880	1.00 19.44	В
MOTA	2313		VAL B		45.996	32.944		1.00 20.38	В
MOTA	2314	C	VAL B		42.723	33.568	7.784		
MOTA	2315	0	VAL B		42.860	34.293	8.766	1.00 19.54	В
ATOM	2316	N	CYS B		41.724	32.701	7.669	1.00 20.87	. В
MOTA	2317	CA	CYS B	117	40.793	32.523	8.774	1.00 22.57	В
MOTA	2318	C	CYS B	117	41.132	31.196	9.444	1.00 21.84	В
MOTA	2319	0	CYS B	117	40.867	30.123	8.892	1.00 22.98	В
MOTA	2320	CB	CYS B	117	39.332	32.486	8.315	1.00 23.53	В
ATOM	2321	SG	CYS B	117	38.217	32.222	9.734	1.00 29.76	В
ATOM	2322	N	SER B	118	41.728	31.277	10.627	1.00 19.87	В
ATOM	2323	CA	SER B		42.094	30.092	11.381	1.00 18.65	В
ATOM	2324	CB	SER B		43.345	30.356	12.226	1.00 19.67	В
	2325	OG	SER B		44.463	30.672	11.421	1.00 22.97	В
ATOM					40.962	29.656	12.300	1.00 18.03	В
MOTA	2326	C	SER B			30.389	13.209	1.00 19.82	В
MOTA	2327	0	SER B		40.579			1.00 17.57	В
ATOM	2328	N	VAL B		40.426	28.463	12.050	1.00 17.37	В
MOTA	2329	CA	VAL B		39.365	27.889	12.874		В
MOTA	2330	CB	VAL B		38.202	27.364	12.006	1.00 15.69	
MOTA	2331		. VAL B		37.091	26.852	12.892	1.00 11.64	В
ATOM	2332	CG2	VAL B	119	37.695	28.484	11.076	1.00 13.82	В
ATOM	2333	C	VAL B	119	40.073	26.739	13.579	1.00 15.38	В
ATOM	2334	0	VAL B	119	40.318	25.680	12.992	1.00 16.76	В
MOTA	2335	N	THR B	120	40.404	26.958	14.844	1.00 16.03	В
MOTA	2336	CA	THR B	120	41.165	25.988	15.615	1.00 15.04	В
ATOM	2337	CB	THR B	120	42.487	26.613	16.031	1.00 13.75	В
ATOM	2338	OG1	THR B	120	42.221	27.713	16.915	1.00 17.84	В
ATOM	2339		THR B		43.230	27.144	14.815	1.00 12.18	В
ATOM	2340	C	THR B		40.533	25.405	16.872	1.00 17.87	В
ATOM	2341	ō	THR B		39.571	25.944	17.425	1.00 17.71	В
ATOM	2342	Ŋ	ASP B		41.132	24.303	17.317	1.00 19.07	В
ATOM	2343	CA	ASP B		40.738	23.576	18.511	1.00 20.97	В
		CB	ASP B		41.268	24.291	19.766	1.00 24.82	В
ATOM	2344		ASP B		42.797	24.330	19.831	1.00 31.04	В
MOTA	2345	CG			43.460	23.360	19.397	1.00 30.81	В
ATOM	2346		L ASP B			25.333	20.346	1.00 34.38	В
ATOM	2347		2 ASP B		43.339			1.00 34.33	В
MOTA	2348	C	ASP B		39.238	23.293	18.679		В
ATOM	2349	0	ASP B		38.629	23.671	19.683	1.00 23.00	
ATOM	2350	N	PHE B	122	38.641	22.613	17.710	1.00 20.38	В
ATOM	2351	CA	PHE B		37.233	22.280	17.818	1.00 18.51	В
ATOM	2352	CB	PHE B	122	36.414	22.988	16.732	1.00 16.18	В
ATOM	2353	CG	PHE B		36.817	22.644	15.319	1.00 13.31	В
MOTA	2354		1 PHE B	122	37.695	23.463	14.615	1.00 11.43	В
ATOM	2355		2 PHE B		36.247	21.547	14.664	1.00 10.93	В
ATOM	2356	-	1 PHE B		37.998		13.272	1.00 10.91	В
ATOM	2357		2 PHE B		36.541		13.317	1.00 12.31	В
ATOM	2358				37.419		12.618	1.00 8.92	В
ATOM	2359		PHE B		37.011		17.739	1.00 19.55	В
ATOM			PHE B		37.889		17.301	1.00 18.45	В
	2360				35.829		18.182	1.00 20.50	В
MOTA	2361		TYR B		35.412		18.180	1.00 21.08	В
MOTA	2362				36.067		19.340	1.00 19.11	В
MOTA	2363	CB	TYR E	143	30.007	40.40L	.J.J40		_

ATOM	2364	CG	TYR B	123	35.919	16.702	19.228	1.00 18.56	В
ATOM	2365		TYR B	127	34.746	16.062	19.629	1.00 19.13	В
									В
ATOM	2366		TYR B		34.572	14.695	19.446	1.00 17.75	
MOTA	2367	CD2	TYR B	123	36.920	15.932	18.647	1.00 17.20	В
ATOM	2368	CE2	TYR B	123	36.762	14.566	18.455	1.00 17.38	В
							18.853	1.00 19.59	В
MOTA	2369	CZ	TYR B		35.584	13.953			
ATOM	2370	OH	TYR B	123	35.412	12.608	18.631	1.00 22.32	В
ATOM	2371	С	TYR B	123	33.896	18.957	18.351	1.00 21.83	В
			•						В
MOTA	2372	0	TYR B	123	33.365	19.708	19.165	1.00 23.26	
ATOM	2373	N	PRO B	124	33.175	18.126	17.584	1.00 21.65	В
ATOM	2374	CD	PRO B	124	31.725	17.996	17.808	1.00 23.81	В
								1.00 22.30	В
MOTA	2375	CA	PRO B		33.627	17.177	16.562		
ATOM	2376	CB	PRO B	124	32.398	16.290	16.353	1.00 21.95	В
ATOM	2377	CG	PRO B	124	31.270	17.237	16.586	1.00 23.07	В
							15.266	1.00 22.20	В
MOTA	2378	C	PRO B		34.128	17.813			
ATOM	2379	0	PRO B	124	34.204	19.035	15.149	1.00 24.43	В
ATOM	2380	N	ALA B	125	34.457	16.971	14.291	1.00 20.63	В
			ALA B		34.987	17.428	13,007	1.00 22.13	В
ATOM	2381	CA							
ATOM	2382	CB	ALA B	125	35.571	16.236	12.244	1.00 20.20	В
MOTA	2383	C	ALA B	125	34.057	18.222	12.078	1.00 22.42	В
MOTA	2384	0	ALA B		34.512	19.129	11.400	1.00 24.48	В
ATOM	2385	N	GLN B	126	32.772	17.893	12.036	1.00 25.59	В
ATOM	2386	CA	GLN B	126	31.845	18.598	11,147	1.00 27.46	В
ATOM	2387	CB	GLN B	126	30.414	18.101	11.357	1.00 29.99	В
								1.00 36.21	В
MOTA	2388	CG	GLN B		30.283	16.595	11.480		
MOTA	2389	CD	GLN B	126	30.625	16.102	12.870	1.00 38.28	В
ATOM	2390	ORI	GLN B	126	30.558	14.905	13.158	1.00 40.46	В
							13.745	1.00 40.92	В
ATOM	2391		GLN B		30.989	17.030			
ATOM	2392	C	GLN B	126	31.876	20.112	11.333	1.00 28.28	В
ATOM	2393	0	GLN B	126	31.571	20.627	12.410	1.00 29.36	В
			ILE B		32.221	20.831	10.273	1.00 27.17	В
ATOM	2394	N							
MOTA	2395	CA	ILE B	127	32.292	22.279	10.353	1.00 27.02	В
MOTA	2396	CB	ILE B	127	33.656	22.716	10.931	1.00 27.21	В
MOTA	2397		ILE B		34.767	22.453	9.898	1.00 21.63	В
								1.00 24.63	В
ATOM	2398		ILE B		33.612	24.195	11.316		
MOTA	2399	CD1	ILE B	127	34.760	24.633	12.198	1.00 25.86	В
ATOM	2400	C	ILE B	127	32.117	22.903	8.969	1.00 27.10	В
						22.258	7.956	1.00 26.58	В
MOTA	2401	0	ILE B		32.393				
ATOM	2402	N	LYS E	128	31.666	24.155	8.940	1.00 25.41	В
MOTA	2403	CA	LYS E	128	31.457	24.884	7.689	1.00 27.45	В
		CB	LYS E		29.964	24.927	7.334	1.00 29.68	В
MOTA	2404								В
ATOM	2405	CG	LYS E	128	29.633	25.685	6.046	1.00 34.69	
ATOM	2406	CD	LYS E	128	30.129	24.954	4.793	1.00 38.25	В
ATOM	2407	CE	LYS E	128	29.802	25.742	3.517	1.00 40.20	В
							2.271	1.00 39.87	В
MOTA	2408	NZ	LYS E		30.281	25.071			
ATOM	2409	C	LYS E	128	31.983	26.301	7.861	1.00 25.41	В
MOTA	2410	0	LYS E	128	31.559	27.019	8.759	1.00 26.68	В
					32.911	26.700	7.002	1.00 25.70	В
MOTA	2411	N	VAL E						
MOTA	2412	CA	VAL E	3 129	33.493	28.034	7.078	1.00 24.82	В
ATOM	2413	CB	VAL E	129	35.013	27.956	7.329	1.00 24.17	В
ATOM	2414		VAL E	120	35.592	29.351	7.452	1.00 22.14	В
								1.00 22.44	В
MOTA	2415	CG2	VAL E		35.295	27.136	8.583		
MOTA	2416	C	VAL I	3 129	33.248	28.791	5.778	1.00 25.17	В
ATOM	2417	0	VAL I	129	33.532	28.283	4.701	1.00 25.50	В
						30.007	5.884	1.00 27.21	В
MOTA	2418	N	ARG I		32.724				
MOTA	2419	CA	ARG I	3 130	32.445	30.814	4.701	1.00 28.49	В
ATOM	2420	CB	ARG 1	3 130	30.931	30.920	4.470	1.00 31.77	В
			ARG I		30.239	29.591	4.183	1.00 34.92	В
MOTA	2421	CG						1.00 41.30	В
MOTA	2422	CD	ARG I	3 130	28.927	29.813	3.432		
MOTA	2423	NE	ARG I	3 130	27.834	30.254	4.291	1.00 42.15	В
ATOM	2424	CZ		3 130	27.032	29.426	4.953	1.00 46.05	В
								1.00 45.50	В
MOTA	2425		L ARG		27.200	28.112	4.849		
ATOM	2426	NH:	2 ARG 1	3 130	26.061	29.910	5.718	1.00 48.30	В
ATOM	2427	C		3 130	33.036	32.211	4.792	1.00 27.57	В
					33.130	32.789	5.874	1.00 26.00	В
MOTA	2428	0		B 130					В
ATOM	2429	N	TRP :	B 131	33.440	32.744	3.645	1.00 27.37	
MOTA	2430	CA	TRP	B 131	34.004	34.085	3.571	1.00 30.27	В
				B 131	35.281	34.083	2.737	1.00 30.21	В
ATOM	2431	CB						1.00 32.32	В
MOTA	2432	CG	TRP :	B 131	36.532	33.844			
MOTA	2433	CD	2 TRP	B 131	37.155	34.757	4.432	1.00 32.41	В
ATOM	2434		2 TRP		38.334		4.900	1.00 33.07	В
							4.897	1.00 31.75	В
MOTA	2435		3 TRP		36.831				
MOTA	2436	CD	1 TRP	B 131	37.333	32.741		1.00 32.80	В
MOTA	2437		1 TRP		38.420	32.913	4.300	1.00 31.53	B
	/								

						24 864	E 010	1 00 22 02	ъ
MOTA	2438		TRP B		39.193	34.764	5.812	1.00 32.82	В
MOTA	2439	CZ3	TRP B	131	37.680	36.656	5.800	1.00 32.08	В
MOTA	2440	CH2	TRP B	131	38.849	36.017	6.249	1.00 33.40	В
ATOM	2441	C	TRP B	131	33.003	35.064	2.949	1.00 32.99	В
ATOM	2442	0	TRP B	131	32.367	34.759	1.940	1.00 32.18	В
ATOM	2443	N	PHE B		32.879	36.242	3.550	1.00 35.48	В
			PHE B			37.263	3.058	1.00 39.35	В
MOTA	2444	CA			31.962				
MOTA	2445	CB	PHE B		30.856	37.501	4.077	1.00 38.14	В
ATOM	2446	CG	PHE B	132	29.843	36.407	4.123	1.00 38.39	В
ATOM	2447	CD1	PHE B	132	28.804	36.373	3.202	1.00 38.31	В
MOTA	2448		PHE B		29.930	35.399	5.075	1.00 38.21	В
ATOM			PHE B		27.860	35.348	3.229	1.00 39.26	В
	2449		PHE B			34.369	5.111	1.00 38.83	В
MOTA	2450				28.992				
MOTA	2451	CZ	PHE B		27.954	34.345	4.184	1.00 37.91	В
MOTA	2452	C	PHE B	132	32.650	38.583	2.755	1.00 41.59	В
MOTA	2453	0	PHE B	132	33.515	39.025	3.508	1.00 42.72	В
ATOM	2454	N	ARG B	133	32.267	39.203	1.640	1.00 45.04	В
ATOM	2455	CA	ARG B		32.829	40.490	1.242	1.00 48.28	В
			ARG B		32.510	40.787	-0.227	1.00 51.68	В
ATOM	2456	CB							В
ATOM	2457	CG	ARG B		33.293	41.958	-0.829	1.00 55.78	
ATOM	2458	CD	ARG B	133	34.787	41.655	-0.867	1.00 57.07	В
ATOM	2459	NE	ARG B	133	35.580	42.741	-1.440	1.00 59.30	В
MOTA	2460	CZ	ARG B	133	35.523	43.135	-2.710	1.00 60.93	В
ATOM	2461	NH1	ARG B	133	34.702	42.536	-3.564	1.00 61.44	В
	2462		ARG B		36.295	44.132	-3.128	1.00 61.77	В
ATOM						41.492	2.145	1.00 49.07	В
ATOM	2463	C	ARG B		32.129				В
MOTA	2464	0	ARG B		32.299	41.460	3.358	1.00 51.26	
ATOM	2465	И	ASN B	134	31.331	42.376	1.572	1.00 49.23	В
ATOM	2466	CA	ASN B	134	30.614	43.336	2.393	1.00 48.83	В
ATOM	2467	CB	ASN B	134	30.582	44.702	1.710	1.00 45.93	В
MOTA	2468	CG	ASN B		31.973	45.290	1.523	1.00 45.10	В
			ASN B		32.450	45.440	0.397	1.00 41.81	В
MOTA	2469							1.00 41.82	В
ATOM	2470		asn b		32.634	45.618	2.634		
ATOM	2471	C	asn b	134	29.203	42.795	2.594	1.00 50.25	В
MOTA	2472	0	asn b	134	28.222	43.529	2.508	1.00 52.28	В
MOTA	2473	N	ASP B	135	29.122	41.496	2.868	1.00 50.15	В
MOTA	2474	CA	ASP B	135	27.847	40.819	3.072	1.00 51.07	В
ATOM	2475	c	ASP B		27.590	39.855	1.910	1.00 51.76	В
ATOM	2476	ō	ASP B		26.586	39.136	1.893	1.00 51.82	В
						39.856	0.944	1.00 50.97	В
ATOM	2477	N	GLN B		28.507				В
MOTA	2478	CA	GLN B		28.421	38.999	-0.240	1.00 51.24	
ATOM	2479	CB	GLN B	136	28.766	39.805	-1.493	1.00 53.78	В
MOTA	2480	CG	GLN B	136	28.736	39.000	-2.783	1.00 58.16	В
ATOM	2481	CD	GLN B	136	29.675	39.559	-3.839	1.00 59.39	В
ATOM	2482	OR1	GLN B	136	30.895	39,527	-3.675	1.00 60.12	В
ATOM	2483		GLN B		29.110	40.078	-4.926	1.00 59.45	В
			GLN B		29.395	37.825	-0.124	1.00 49.46	В
MOTA	2484	C					-0.035	1.00 48.29	В
MOTA	2485	0	GLN B		30.607	38.026			
MOTA	2486	N	GLU B		28.873	36.603	-0.144	1.00 47.64	В
MOTA	2487	CA	GLU B	137	29.730	35.432	-0.027	1.00 46.85	В
MOTA	2488	CB	GLU B	137	28.899	34.152	0.022	1.00 47.17	В
ATOM	2489	CG	GLU B	137	29.695	32.975	0.556	1.00 50.22	В
ATOM	2490	CD	GLU B		28.866	31.726	0.743	1.00 52.65	В
ATOM	2491		GLU B		27.699	31.842	1.171	1.00 55.57	В
					29.391	30.623	0.478	1.00 54.41	В
MOTA	2492		GLU B					1.00 45.23	В
MOTA	2493	С	GLU B		30.755	35.320	-1.149		
MOTA	2494	0	GLU B	137	30.445	35.544	-2.314	1.00 45.04	В
ATOM	2495	N	GLU B	138	31.983	34.977	-0.776	1.00 44.63	В
MOTA	2496	CA	GLU E	138	33.078	34.808	-1.724	1.00 44.36	В
ATOM	2497	СВ	GLU B	138	34.284	35.658	-1.307	1.00 45.65	В
		CG	GLU E		34.076	37.166	-1.320	1.00 48.42	В
ATOM	2498					37.761	-2.717	1.00 50.71	В
MOTA	2499	CD	GLU E		34.144			1.00 51.60	В
MOTA	2500		. GLU E		35.120	37.471	-3.442		
ATOM	2501	OE2	GLU E		33.227	38.526	-3.086	1.00 50.99	В
ATOM	2502	C	GLU E	138	33.498	33.335	-1.740	1.00 43.68	B
ATOM	2503	0	GLU E	138	33.831	32.769	-0.697	1.00 43.53	В
ATOM	2504	N	THR E		33.468	32.711	-2.914	1.00 42.58	В
ATOM	2505	CA	THR E		33.881		-3.044	1.00 41.76	В
					32.739	30.415	-3.543	1.00 41.04	В
MOTA	2506	CB	THRE				-4.759	1.00 40.71	В
MOTA	2507		L THR E		32.207			1.00 41.89	В
MOTA	2508		? THR E		31.641		-2.492		
MOTA	2509	C	THR I	3 139	35.038		-4.026		В
ATOM	2510	0	THR E	3 139	35.855	30.326	-3.981		В
MOTA	2511	N	ALA I	3 140	35.096	32.224	-4.920	1.00 40.67	В

3.004	0510	~	ALA B	140	36.179	32.305	-5.887	1.00 41.22	В
MOTA	2512	CA						1.00 41.13	В
ATOM	2513	CB	ALA B		35.714	33.016	-7.158		
MOTA	2514	C	ALA B		37.247	33.126	-5.177	1.00 41.09	В
MOTA	2515	0	ALA B	140	36.976	34.232	-4.693	1.00 43.11	В
ATOM	2516	N	GLY B	141	38.455	32.582	-5.102	1.00 39.60	В
ATOM	2517	CA	GLY B	141	39.526	33.278	-4.418	1.00 35.11	В
ATOM	2518	C	GLY B	141	39.739	32,651	-3.051	1.00 33.42	В
ATOM	2519	ō	GLY B		40.605	33.076	-2.287	1.00 31.24	В
							-2.750	1.00 31.89	В
ATOM	2520	N	VAL B		38.945	31.628			
ATOM	2521	CA	VAL B		39.033	30.937	-1.470	1.00 32.27	В
ATOM	2522	CB	VAL B	142	37.645	30.790	-0.813	1.00 31.90	В
ATOM	2523	CG1	VAL B	142	37.733	29.861	0.400	1.00 32.37	В
ATOM	2524	CG2	VAL B	142	37.125	32.161	-0.402	1.00 32.53	В
ATOM	2525	C	VAL B		39.652	29.552	-1.564	1.00 31.26	В
		ō	VAL B		39.211	28.712	-2.343	1.00 32.44	В
ATOM	2526								В
ATOM	2527	N	VAL B		40.676	29.326	-0.752	1.00 30.76	
MOTA	2528	CA	VAL B		41.357	28.045	-0.702	1.00 29.79	В
ATOM	2529	CB	VAL B	143	42.815	28.154	-1.162	1.00 29.63	В
ATOM	2530	CG1	VAL B	143	43.439	26.768	-1.212	1.00 31.60	В
ATOM	2531	CG2	VAL B	143	42.885	28.819	-2.514	1.00 33.43	В
ATOM	2532	C	VAL B	143	41.357	27.575	0.749	1.00 30.61	В
ATOM	2533	ō	VAL B		41.665	28.338	1.667	1.00 28.64	В
						26.313	0.950	1.00 29.65	В
ATOM	2534	N	SER B		41.017				
ATOM	2535	CA	SER B		40.970	25.756	2.282	1.00 28.42	В
MOTA	2536	CB	SER B	144	39.541	25.325	2.605	1.00 29.23	В
MOTA	2537	OG	SER B	144	39.457	24.705	3.875	1.00 33.81	В
MOTA	2538	C	SER B	144	41.900	24.562	2.373	1.00 27.32	В
ATOM	2539	0	SER B	144	42.101	23.840	1.397	1.00 27.40	В
ATOM	2540	N	THR B		42.492	24.372	3.542	1.00 25.70	В
			THR B		43.364	23.227	3.755	1.00 24.82	В
MOTA	2541	CA						1.00 25.01	В
MOTA	2542	CB	THR B		44.272	23.418	4.995		
ATOM	2543	OG1	THR B		43.467	23.399	6.186	1.00 25.18	В
MOTA	2544	CG2	THR B	145	45.022	24.743	4.923	1.00 23.27	В
MOTA	2545	С	THR B	145	42.392	22.100	4.071	1.00 24.16	В
ATOM	2546	0	THR B	145	41.200	22.335	4.272	1.00 23.86	В
ATOM	2547	N	PRO B		42.865	20.854	4.081	1.00 23.17	В
						20.231	3.618	1.00 22.29	В
MOTA	2548	СD	PRO E		44.116				
MOTA	2549	CA	PRO E		41.854	19.852	4.419	1.00 23.18	В
MOTA	2550	CB	PRO E	146	42.521	18.536	4.008	1.00 24.20	В
MOTA	2551	CG	PRO E	146	43.998	18.833	4.162	1.00 22.82	В
ATOM	2552	С	PRO E	146	41.597	19.945	5.933	1.00 22.63	В
ATOM	2553	0	PRO E	146	42.213	20.766	6.625	1.00 21.32	В
ATOM	2554	N	LEU E		40.667	19.146	6.445	1.00 22.60	В
					40.414	19.142	7.883	1.00 22.34	В
ATOM	2555	CA	LEU E						В
MOTA	2556	CB	LEU E		39.241	18.216	8,213	1.00 22.17	
MOTA	2557	CG	TEO E	3 147	38.934	17.973	9.691	1.00 24.53	В
ATOM	2558	CD1	LEU E	3 147	38.629	19.288	10.368	1.00 25.95	В
ATOM	2559	CD2	LEU E	3 147	37.746	17.026	9.826	1.00 25.55	В
ATOM	2560	C	LEU E	3 147	41.710	18.609	8.515	1.00 21.99	В
MOTA	2561	ō	LEU I		42.290	17.640	8.024	1.00 21.35	В
			ILE		42.175	19.246	9.581	1.00 20.48	В
MOTA	2562	N						1.00 19.15	В
MOTA	2563	CA	ILE E		43.406	18.813	10.228		
MOTA	2564	СВ	ILE E		44.392	19.990	10.403	1.00 21.68	В
MOTA	2565	CG2	: ILE P	3 148	45.666	19.505	11.065	1.00 20.10	В
MOTA	2566	CGI	ILE F	3 148	44.728	20.609	9.041	1.00 25.04	В
ATOM	2567	CD1	ILE E	3 148	45.416	19.649	8.090	1.00 29.06	В
MOTA	2568	C		3 148	43.160	18.208	11.603	1.00 17.56	В
	2569	ŏ		B 148	42.566	18,852	12.467	1.00 14.88	В
MOTA			ARG I				11.795	1.00 15.95	В
MOTA	2570	N			43.625	16.973			
MOTA	2571	CA	ARG I		43.492	16.273	13.077	1.00 17.47	. B
ATOM	2572	CB	ARG I	B 149	43.420	14.763	12.852	1.00 16.94	В
ATOM	2573	CG	ARG I	B 149	43.202	13.941	14.128	1.00 20.29	В
MOTA	2574	CD	ARG 1	B 149	43.252	12.448	13.821	1.00 21.64	В
ATOM	2575	NE		B 149	42,168	12.028	12.938	1.00 21.97	В
		CZ		B 149	40.934	11.742	13.348	1.00 23.22	В
MOTA	2576					11.374	12.471	1.00 23.89	В
ATOM	2577		L ARG		40.015			1.00 23.03	В
MOTA	2578		2 ARG		40.623	11.803	14.636		
MOTA	2579	C		B 149	44.720	16.603	13.937	1.00 17.66	В
MOTA	2580	0	ARG	B 149	45.850	16.311	13.549	1.00 17.51	В
ATOM	2581	N	ASN	B 150	44.496	17.210	15.098	1.00 16.67	В
ATOM	2582	CA		B 150	45.592	17.593	15.980	1.00 16.94	В
MOTA	2583	CB		B 150	45.174	18.756	16.890	1.00 15.38	В
				B 150	44.899	20.034	16.118	1.00 18.41	В
ATOM	2584	CG						1.00 19.05	В
MOTA	2585	OD	1 ASN	טבג פ	45.685	20.436	15.249	2.00 23.03	

ATOM	2586	ND2	ASN B	150	43.790	20.691	16.440	1.00 17.88	В
ATOM	2587	C	ASN B	150	46.116	16.452	16.841	1.00 18.47	В
MOTA	2588	0	asn b		47.220	16.540	17.384	1.00 17.03	В
MOTA	2589	N	GLY B		45.324	15.391	16.968	1.00 17.77	В
MOTA	2590	CA	GLY B		45.734	14.251	17.770	1.00 19.16	В
MOTA	2591	C	GLY B		45.258	14.293	19.213	1.00 20.44	B B
ATOM	2592	0	GLY B ASP B		45.198 44.906	13.264 15.475	19.877 19.701	1.00 20.79	В
ATOM ATOM	2593 2594	N CA	ASP B		44.450	15.624	21.077	1.00 21.97	В
ATOM	2595	CB	ASP B		45.192	16.790	21.748	1.00 21.95	В
ATOM	2596	CG	ASP B		45.027	18.101	20.992	1.00 28.05	В
ATOM	2597		ASP B		45.764	19.060	21.300	1.00 30.94	В
ATOM	2598		ASP B		44.158	18.181	20.090	1.00 28.02	В
ATOM	2599	C	ASP B	152	42.939	15.847	21.175	1.00 20.51	В
ATOM	2600	0	ASP B	152	42.474	16.619	22.010	1.00 21.63	В
ATOM	2601	N	TRP B	153	42.183	15.166	20.322	1.00 19.19	В
MOTA	2602	CA	TRP B		40.724	15.278	20.300	1.00 16.82	В
ATOM	2603	СВ	TRP B		40.121	14.865	21.657	1.00 15.80	В
ATOM	2604	CG	TRP B		40.326	13.408	22.005	1.00 16.21	В
ATOM	2605		TRP B		39.415	12.322	21.756	1.00 16.58 1.00 15.08	B B
MOTA	2606	CE2	TRP B		40.047 38.125	11.134 12.238	22.188	1.00 15.69	В
ATOM ATOM	2607 2608	CE3	TRP B		41.435	12.848	22.564	1.00 14.68	В
ATOM	2609		TRP B		41.278	11.483	22.677	1.00 15.53	В
ATOM	2610		TRP B		39.438	9.879	22.087	1.00 15.60	В
ATOM	2611			153	37.518	10.987	21.112	1.00 14.22	В
ATOM	2612	CH2	TRP B	153	38.176	9.827	21.549	1.00 13.89	В
ATOM	2613	C	TRP B	153	40.194	16.660	19.890	1.00 16.09	В
ATOM	2614	0	TRP B	153	39.159	17.110	20.379	1.00 14.28	В
MOTA	2615	N	THR B		40.929	17.342	19.020	1.00 15.11	В
MOTA	2616	CA	THR B		40.499	18.627	18.483	1.00 16.19	В
ATOM	2617	CB	THR B		41.176	19.877	19.150	1.00 18.02	B B
ATOM	2618		THR B		42.602	19.804 20.000	19.008 20.608	1.00 19.50 1.00 15.03	В
ATOM ATOM	2619 2620	CG2	THR B		40.788 40.908	18.602	17.024	1.00 15.05	В
ATOM	2621	0	THR B		41.773	17.832	16.635	1.00 15.24	В
ATOM	2622	N	PHE B		40.269	19.437	16.220	1.00 18.04	В
ATOM	2623	CA	PHE B		40.577	19.538	14.801	1.00 16.03	В
ATOM	2624	CB	PHE B	155	39.404	19.042	13.938	1.00 16.98	В
MOTA	2625	CG	PHE B		39.069	17.579	14.118	1.00 17.58	В
MOTA	2626		PHE B		38.133	17.170	15.074	1.00 18.20	В
MOTA	2627		PHE B		39.670	16.611	13.312	1.00 17.71 1.00 17.81	B
MOTA	2628	CE1	PHE B		37.799 39.346	15.810 15.250	15.223 13.451	1.00 17.57	В
ATOM ATOM	2629 2630	CZ	PHE B		38.407	14.849	14.409	1.00 16.39	В
ATOM	2631	C	PHE B		40.793	21.015	14.503	1.00 16.67	В
ATOM	2632	ŏ	PHE B		40.532	21.870	15.352	1.00 16.84	В
ATOM	2633	N	GLN B		41.281	21.312	13.304	1.00 14.72	В
ATOM	2634	CA	GLN B	156	41.467	22.689	12.886	1.00 14.66	В
MOTA	2635	CB	GLN B	156	42.811	23.264	13.357	1.00 16.69	В
MOTA	2636	CG	GLN B		44.039	22.698	12.669	1.00 15.65	В
MOTA	2637	CD	GLN B		45.292	23.486	13.011	1.00 17.87	В
MOTA	2638		GLN B		45.477	24.617	12.555	1.00 17.56	В
MOTA	2639		GLN B		46.153	22.897	13.830 11.371	1.00 15.40 1.00 14.00	B B
MOTA	2640 2641	0	GLN B		41.398 41.477	22.722 21.691	10.716	1.00 15.17	В
MOTA MOTA	2642	N	ILE B		41.241	23.911	10.818	1.00 15.34	В
MOTA	2643	CA	ILE B		41.165	24.057	9.383	1.00 17.26	В
ATOM	2644	CB	ILE B		39.791	23.585	8.856	1.00 16.56	В
ATOM	2645		ILE B		38.675	24.429	9.474	1.00 13.07	В
MOTA	2646		L ILE B		39.765	23.649	7.326	1.00 17.72	В
MOTA	2647	CD	L ILE E	157	38.583	22.913	6.712	1.00 14.50	В
MOTA	2648	C	ILE P		41.379	25.523	9.074	1.00 18.67	В
ATOM	2649	0	ILE E		40.823	26.391	9.745	1.00 22.28	В
MOTA	2650	N	LEU E		42.217	25.795	8.083 7.690	1.00 18.98 1.00 20.77	B
MOTA	2651	CA	LEU E		42.508 44.022	27.162 27.368	7.555	1.00 20.77	В
MOTA	2652 2653	CB CG	TEO E		44.851	27.525	8.838	1.00 26.12	В
ATOM ATOM	2654		L LEU E		44.689	26.320	9.740	1.00 29.01	В
MOTA	2655		LEU E		46.311	27.701	8.465	1.00 28.46	В
MOTA	2656	C	LEU E		41.817	27.484	6.371	1.00 20.61	В
ATOM	2657	0	LEU E	3 158	41.934	26.734	5.401	1.00 19.39	В
MOTA	2658	N	VAL I		41.088	28.596	6.346	1.00 21.67	В
MOTA	2659	CA	VAL I	159	40.380	29.011	5.141	1.00 21.90	В

ATOM	2660	СВ	VAL B	150	38.855	29.061	5.365	1.00 22.06	В
						29.252		1.00 20.55	В
ATOM	2661		VAL B		38.147		4.043		
ATOM	2662		VAL B		38.381	27.766	6.009	1.00 20.83	В
MOTA	2663	C	VAL B	159	40.899	30.379	4.749	1.00 21.80	В
ATOM	2664	0	VAL B	159	40.721	31.357	5.473	1.00 20.82	В
MOTA	2665	N	MET B	160	41.555	30.416	3.592	1.00 23.56	В
ATOM	2666	CA	MET B	160	42.179	31.613	3.055	1.00 25.12	В
ATOM	2667	CB	MET B		43.580	31.257	2.559	1.00 26.80	В
		CG	MET B		44.479	30.736	3.678	1.00 32.00	В
MOTA	2668								В
MOTA	2669	SD	MET B		45.850	29.700	3.145	1.00 38.02	
MOTA	2670	CE	MET B	160	45.094	28.065	3.307	1.00 35.43	В
MOTA	2671	С	MET B	160	41.387	32.269	1.941	1.00 28.27	В
ATOM	2672	0	MET B	160	40.684	31.602	1.177	1.00 28.76	В
ATOM	2673	N	LEU B		41.518	33.588	1.854	1.00 29.59	В
ATOM	2674	CA	LEU B		40.820	34.366	0.845	1.00 32.69	В
			PEO B		39.669	35.142	1.487	1.00 30.80	В
ATOM	2675	CB					0.586		В
MOTA	2676	CG	PEA B		39.031	36.199		1.00 31.56	
MOTA	2677		LEU B		38.156	35.516	-0.460	1.00 29.64	В
MOTA	2678	CD2	LEU B	161	38.213	37.167	1.423	1.00 29.89	В
MOTA	2679	Ċ	LEU B	161	41.755	35.349	0.154	1.00 35.59	В
ATOM	2680	0	LEU B	161	42.350	36.216	0.801	1.00 35.54	В
MOTA	2681	N	GLU B		41.895	35.203	-1.158	1.00 39.87	В
ATOM	2682	CA	GLU B		42.728	36.118	-1.927	1.00 44.05	В
		CB	GLU B		42.995	35.565	-3.331	1.00 46.86	В
MOTA	2683							1.00 50.98	В
ATOM	2684	CG	GLU B		43.795	36.497	-4.239		
MOTA	2685	CD	GLO B		45.274	36.537	-3.891	1.00 54.75	В
MOTA	2686	OEl	GLU B	162	45.604	36.802	-2.715	1.00 56.53	В
ATOM	2687	OE2	GLU B	162	46.108	36.308	-4.796	1.00 55.16	В
ATOM	2688	C	GLU B	162	41.879	37.372	-2.029	1.00 44.69	В
ATOM	2689	Ó	GLU B	162	40.719	37.302	-2.434	1.00 44.39	В
ATOM	2690	N	MET B		42.436	38.514	-1.648	1.00 46.67	В
					41.670	39.746	-1.716	1.00 49.56	В
MOTA	2691	CA	MET B						В
MOTA	2692	CB	MET B		40.881	39.949	-0.412	1.00 51.22	
ATOM	2693	CG	MET B	163	41.652	39.675	0.876	1.00 51.58	В
MOTA	2694	SD	MET B	163	42.910	40.901	1.274	1.00 56.87	В
MOTA	2695	CE	MET B	163	41.915	42.187	2.029	1.00 54.89	В
ATOM	2696	C	MET B	163	42.487	40.986	-2.028	1.00 51.43	В
ATOM	2697	ō	MET B		43.717	40.988	-1.942	1.00 51.02	В
ATOM	2698	N	THR B		41.777	42.038	-2.412	1.00 53.70	В
					42.385	43.316	-2.738	1.00 56.61	В
ATOM	2699	CA	THR B						В
ATOM	2700	CB	THR B		41.889	43.820	-4.116	1.00 57.48	
ATOM	2701	OG1			40.457	43.744	-4.172	1.00 57.81	В
MOTA	2702	CG2	THR B	164	42.480	42.967	-5.234	1.00 57.23	В
ATOM	2703	C	THR B	164	42.012	44.318	-1.642	1.00 57.80	В
ATOM	2704	0	THR B	164	40.866	44.766	-1.555	1.00 57.08	В
ATOM	2705	N	PRO E		42.976	44.658	-0.770	1.00 58.98	В
MOTA	2706	CD	PRO E		44.315	44.055	-0.647	1.00 59.54	В
					42.734	45.605	0.322	1.00 60.52	В
MOTA	2707	CA	PRO E						В
ATOM	2708	CB	PRO E		44.063	45.608	1.078	1.00 60.33	
MOTA	2709	CG	PRO E	165	44.604	44.236	0.822	1.00 60.42	В
ATOM	2710	C	PRO E	165	42.347	47.002	-0.163	1.00 61.65	В
ATOM	2711	0	PRO E	165	43.149	47.698	-0.790	1.00 61.24	В
MOTA	2712	N	GLN F	166	41.110	47.395	0.126	1.00 62.45	В
ATOM	2713	CA	GLN F		40.598	48.709	-0.250	1.00 63.32	В
MOTA	2714	СВ	GLN E		39.605	48.590	-1.410	1.00 65.46	В
			GLN E		40.177	47.945	-2.661	1.00 69.00	В
MOTA	2715	CG				47.942	-3.819	1.00 71.19	В
MOTA	2716	CD	GTN E		39.195				
MOTA	2717		GLN E		38.071	47.448	-3.697	1.00 72.48	В
MOTA	2718	NE2	GLN I	3 166	39.617	48.492	-4.954	1.00 72.65	В
ATOM	2719	С	GLN I	3 166	39.893	49.287	0.970	1.00 62.65	В
MOTA	2720	0	GLN I	3 166	39.021	48.635	1.550	1.00 62.16	, в
ATOM	2721	N		3 167	40.266	50.501	1.366	1.00 61.62	В
MOTA	2722	CA		3 167	39.645	51.111	2.535	1.00 60.86	В
			-	B 167	40.190	52.525	2.777	1.00 62.57	В
ATOM	2723	CB						1.00 64.82	В
ATOM	2724	CG		B 167	39.953	53.029	4.204		
ATOM	2725	æ		B 167	40.742	52.198	5.227	1.00 67.31	В
MOTA	2726	NE		B' 167	40.094	52.143	6.539	1.00 69.03	В
MOTA	2727	CZ		B 167	40.570	51.477	7.591	1.00 69.14	В
ATOM	2728	NHI	ARG 1	B 167	41.710	50.804	7.499	1.00 69.34	В
ATOM	2729		ARG		39.897		8.735	1.00 69.52	В
ATOM	2730	C		B 167	38.136		2.333	1.00 59.19	В
		Ö		B 167	37.647		1.303	1.00 58.60	В
MOTA	2731						3.320	1.00 58.18	В
ATOM	2732	N		B 168	37.404			1.00 56.57	В
MOTA	2733	ÇA	ا لابلاق	B 168	35.959	50,632	3.226	2.00 50.57	•

ATOM	2734	C	GLY B 1	L68	35.466	49.200	3.191	1.00 55.42	В
ATOM	2735	0	GLY B 1	L68	34.306	48.924	3.495	1.00 55.98	В
ATOM	2736	N	ASP B 1		36.350	48.280	2.814	1.00 53.44	В
						46.871	2.757	1.00 51.76	В
ATOM	2737	CA	ASP B 1		35.979				
MOTA	2738	CB	ASP B 1	L69	36.841	46.115	1.740	1.00 50.49	В
ATOM	2739	CG	ASP B 1	L69	36.428	46.392	0.311	1.00 50.57	В
ATOM	2740	OD1	ASP B 1	169	35.207	46.479	0.060	1.00 49.92	B
ATOM	2741		ASP B 1		37.318	46.507	-0.559	1.00 49.84	В
						46.181	4.110	1.00 49.36	В
ATOM	2742	C	ASP B 1		36.083				
ATOM	2743	0	ASP B	169	37.066	46.343	4.836	1.00 48.92	В
MOTA	2744	N	VAL B 1	1.70	35.047	45.418	4.436	1.00 47.48	В
ATOM	2745	CA	VAL B 1	170	34.981	44.667	5.680	1.00 45.10	В
ATOM	2746	CB	VAL B	170	33.800	45.130	6.543	1.00 45.86	В
			VAL B		33.702	44.268	7.795	1.00 46.26	В
ATOM	2747							1.00 46.23	В
MOTA	2748	CG2	VAL B		33.974	46.598	6.906		
ATOM	2749	С	VAL B	170	34.787	43.191	5.342	1.00 43.62	В
ATOM	2750	0	VAL B :	170	33.774	42.807	4.762	1.00 42.86	В
MOTA	2751	N	TYR B	171	35.762	42.367	5.704	1.00 41.69	В
ATOM	2752	CA	TYR B		35.694	40.935	5.425	1.00 38.95	В
						40.455	4.899	1.00 37.52	В
MOTA	2753	CB	TYR B		37.044				
MOTA	2754	CG	TYR B	171	37.405	41.031	3.553	1.00 38.12	В
MOTA	2755	CD1	TYR B	171	37.023	40.391	2.376	1.00 37.52	В
MOTA	2756	CEL	TYR B	171	37.342	40.923	1.131	1.00 38.06	В
ATOM	2757	CD2			38.118	42,224	3.454	1.00 37.54	В
					38.442	42.767	2.216	1.00 38.45	В
ATOM	2758	CE2							В
ATOM	2759	\mathbf{cz}	TYR B		38.052	42.110	1.056	1.00 39.25	
ATOM	2760	OH	TYR B	171	38.372	42.641	-0.172	1.00 38.84	В
ATOM	2761	С	TYR B	171	35.314	40.139	6.671	1.00 37.46	В
MOTA	2762	0	TYR B	171	35.791	40.428	7.773	1.00 34.85	В
ATOM	2763	N	THR B		34.452	39.140	6.501	1.00 35.06	В
						38.328	7.638	1.00 35.81	В
ATOM	2764	CA	THR B		34.049				
ATOM	2765	CB	THR B		32.589	38.622	8.064	1.00 38.37	В
ATOM	2766	OG1	THR B	172	31.688	38.177	7.043	1.00 42.02	В
ATOM	2767	CG2	THR B	172	32.390	40.119	8.292	1.00 39.83	В
MOTA	2768	C	THR B	172	34.182	36.830	7.406	1.00 33.71	В
		ō	THR B		33.953	36.335	6.300	1.00 32.99	В
ATOM	2769						8.463	1.00 32.09	В
ATOM	2770	N	CYS B		34.578	36.123			
ATOM	2771	CA	CYS B	173	34.714	34.670	8.438	1.00 31.08	В
ATOM	2772	С	CYS B	173	33.497	34.183	9.200	1.00 30.92	В
MOTA	2773	0	CYS B	173	33.240	34.614	10.326	1.00 32.70	В
MOTA	2774	СВ	CYS B		35.988	34.214	9.155	1.00 31.48	В
			CYS B		36.338	32.436	8.983	1.00 31.85	В
MOTA	2775	SG					8.578	1.00 30.26	В
ATOM	2776	N	HIS B		32.748	33.288			
MOTA	2777	CA	HIS B	174	31.524	32.754	9.152	1.00 29.72	В
ATOM	2778	CB	HIS B	174	30.401	32.977	8.128	1.00 30.80	В
MOTA	2779	CG	HIS B	174	29.030	32.625	8.615	1.00 32.90	В
ATOM	2780		HIS B		28.016	33.405	9.058	1.00 33.11	В
			HIS B		28.551	31.332	8.621	1.00 34.85	В
MOTA	2781							1.00 37.21	В
ATOM	2782		HIS B		27.299	31.332	9.044		
MOTA	2783	NE	HIS B	174	26.950	32.577	9.316	1.00 34.95	В
ATOM	2784	C	HIS B	174	31.751	31.271	9.449	1.00 28.49	В
ATOM	2785	0	HIS B	174	32.080	30.494	8.554	1.00 27.69	В
ATOM	2786	N	VAL B		31.584	30.888	10.710	1.00 27.48	В
	2787	CA	VAL B		31.810	29.508	11.121	1.00 25.94	В
MOTA								1.00 25.31	В
MOTA	2788	CB	VAL B		32.988	29.418	12.126		
MOTA	2789	CG:	L VAL B	175	33.147	27.982	12.629	1.00 21.10	В
MOTA	2790	CG:	VAL B	175	34.271	29.896	11.462	1.00 22.12	В
MOTA	2791	C	VAL B	175	30.606	28.821	11.748	1.00 26.58	В
ATOM	2792	0	VAL B		30.004	29.328	12.694	1.00 27.01	В
		N	GLU B		30.274	27.652	11.212	1.00 27.17	В
MOTA	2793						11.712	1.00 28.51	В
MOTA	2794	CA	GLU B		29.168	26.846			
MOTA	2795	CB	GLU B		28.166	26.573	10.588	1.00 32.35	В
ATOM	2796	CG	GLU B	176	27.454	27.827	10.082	1.00 38.87	В
MOTA	2797	CD	GLU B	176	26.776	27.616	8.735	1.00 42.45	В
ATOM	2798		1 GLU B		25.947	26.684	8.618	1.00 43.07	В
	2799				27.075	28.386	7.794	1.00 42.94	В
MOTA							12.235	1.00 27.34	В
MOTA	2800		GLU B		29.750	25.536			В
MOTA	2801		GLU B		30.576	24.900	11.574	1.00 26.12	
MOTA	2802	N	HIS B	177	29.308	25.134	13.420	1.00 26.08	В
MOTA	2803	CA	HIS B	177	29.800	23.921	14.049	1.00 26.30	В
ATOM	2804				31.132	24.244	14.738	1.00 24.58	В
MOTA	2805				31.759		15.422	1.00 22.32	В
						_	14.977	1.00 21.05	В
MOTA	2806		2 HIS B		32.646		16.710	1.00 21.01	В
MOTA	2807	ND	1 HIS B	177	31.437	22.711	10.710	T.00 ET.01	

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	W	O 03/096	984								
E.	ATOM	2808	CB1	HIS	В	177	32.097	21.613	17.030	1.00 23.72	В
	ATOM			HIS			32.838	21.255	15.995	1.00 23.87	В
	ATOM		C	HIS			28.762	23.413	15.057	1.00 27.87	В
	ATOM		0	HIS			28.059	24.205 22.085	15.672 15.237	1.00 29.54 1.00 29.57	B
	ATOM		CD M	PRO PRO			28.654 29.365	21.025	14.501	1.00 28.96	В
	ATOM ATOM		CA	PRO			27.687	21.497	16.175	1.00 31.71	В
	ATOM		CB	PRO			28.062	20.019	16.166	1.00 30.49	В
	ATOM		CG	PRO	В	178	28.503	19.810	14.769	1.00 30.01	В
•	MOTA		C			178	27.649	22.071	17.595	1.00 33.29 1.00 35.00	B B
	ATOM		0			178 179	26.619 28.762	22.020 22.615	18.256 18.067	1.00 34.96	В
. 3	ATOM ATOM		n Ca			179	28.813	23.168	19.418	1.00 36.85	В
	ATOM		CB			179	30.261	23.228	19.896	1.00 35.35	В
•	MOTA		OG	SER	В	179	31.023	24.053	19.034	1.00 35.14	В
	MOTA		C			179	28.206	24.564	19.522	1.00 38.40	B B
	MOTA		0			179	27.953 27.971	25.056 25.192	20.619 18.377	1.00 37.27 1.00 40.10	В
	MOTA MOTA		n Ca			180 180	27.434	26.545	18.340	1.00 41.36	В
•	ATOM		CB			180	28.162	27.352	17.269	1.00 39.74	В
	ATOM	2828	CG	LEU	В	180	29.677	27.432	17.422	1.00 39.93	В
	MOTA			LEU			30.286	28.013	16.157	1.00 39.41 1.00 39.61	B B
	MOTA			LEU		180 180	30.021 25.944	28.279 26.633	18.636 18.078	1.00 43.85	В
	MOTA MOTA		C 0			180	25.449	26.125	17.072	1.00 44.25	В
	ATOM		N			181	25.230	27.289	18.984	1.00 47.20	В
	ATOM		CA			181	23.794	27.475	18.814	1.00 49.93	В
	ATOM	2835	CB			181	23.158	27.956	20.121	1.00 52.00 1.00 56.40	B B
	ATOM	2836	CG			181	23.873	29.134 29.538	20.758 22.084	1.00 59.03	В
	MOTA MOTA	2837 2838	CD			181	22.087	29.908	22.153	1.00 60.55	В
	ATOM					181	24.059	29.468	23.149	1.00 58.44	В
_	MOTA	2840	C	GLN	В	181	23.635	28.522	17.715	1.00 49.23	В
•	MOTA	2841	0			181	22.712	28.465	16.906	1.00 49.91 1.00 48.48	B B
	MOTA	2842	N			182 182	24.560 24.555	29.474 30.523	17.688 16.679	1.00 47.89	В
	MOTA MOTA	2843 2844	CA CB			182	24.241	31.879	17.314	1.00 48.68	В
	ATOM	2845	OG			182	25.211	32.223	18.286	1.00 50.58	В
•	ATOM	2846	C	SER	В	182	25.938	30.550	16.038	1.00 45.93	В
•	MOTA	2847	0			182	26.945	30.354	16.714	1.00 45.13 1.00 45.12	B B
	ATOM	2848	CD N			183 183	26.004 24.911	30.783 31.096	14.721 13.784	1.00 44.93	В
	MOTA MOTA	2849 2850	CA			183	27.302	30.819	14.042	1.00 43.29	В
	ATOM	2851	СВ			183	26.923	31.070	12.581	1.00 43.70	В
	ATOM	2852	CG			183	25.642	31.833	12.688	1.00 44.70	В
	ATOM	2853	C			3 183	28.254	31.876	14.593 15.209	1.00 40.67 1.00 40.46	B B
	MOTA	2854	и 0			3 183 3 184	27.828 29.547	32.851 31.664	14.382	1.00 40.46	В
•	MOTA MOTA	2855 2856	CA			3 184	30.550	32.607	14.842	1.00 35.88	В
	ATOM	2857	СВ			3 184	31.759	31.889	15.468	1.00 35.92	В
•	MOTA	2858	CG2	ILE	Z	3 184	32.907	32.867	15.657	1.00 35.57	В
	MOTA	2859				3 184	31.362	31.270 30.477	16.806 17.458	1.00 36.74 1.00 36.59	B B
	MOTA	2860	CD:			B 184 B 184	32.475 31.040	30.477	13.680	1.00 34.88	В
	MOTA MOTA	2861 2862	0			B 184	31.412	32.932	12.630	1.00 35.06	В
	ATOM	2863	И			B 185	31.043	34.764	13.876		В
	ATOM	2864	CA			B 185	31.500	35.675		1.00 34.32	В
	MOTA	2865	CB			B 185	30.356	36.592 37.285			B
	MOTA	2866				B 185 B 185	29.770 29.286				В
	MOTA MOTA	2867 2868	C			B 185	32.622	_			В
٠.	MOTA	2869	ŏ			B 185	32.559	37.050	14.494	1.00 32.86	В
	MOTA	2870	N	VA	L	B 186	33.652				В
	MOTA	2871	CA			B 186	34.791				B
	MOTA	2872	CB			B 186	36.041 37.212				В
	MOTA MOTA	2873 2874				B 186 B 186	37.212				В
	ATOM	2875	C			B 186	35.023	38.454	11.721	1.00 34.68	В
	ATOM	2876	ō	VA	L	B 186	35.060				В
	ATOM	2877	N			B 187	35.172				B B
	MOTA	2878	CA			B 187	35.373 34.484				В
	mota Mota	2879 2880	CE			B 187 B 187	33.008				В
	ATOM	2881	CE			B 187	32.146				В
	200 011				_						

ATOM	2882	OE1	GLU B	1	87	30.909	42.739	11.545	1.00		В
ATOM	2883		GLU E			32.701	43.997	11.363	1.00		В
ATOM	2884	C	GLU E			36.816	41.175 40.998	10.784 11.684	1.00		B B
MOTA MOTA	2885 2886	O N	GLU P			37.637 37.113	41.765	9.635	1.00		В
ATOM	2887	CA	TRP E			38.430	42.302	9.360	1.00		В
ATOM	2888	СВ	TRP E			39.339	41.252	8.736	1.00	38.70	В
ATOM	2889	CG	TRP E	3 1	88	40.769	41.704	8.693	1.00	37.82	В
ATOM	2890	CD2	TRP F	3 1	88	41.421	42.383	7.615	1.00		В
MOTA	2891	CE2				42.748	42.640	8.023	1.00		В
ATOM	2892	CE3				41.013	42.799	6.340 9.686	1.00		B B
ATOM	2893		TRP F			41.698 42.890	41.583 42.141	9.291	1.00		В
ATOM ATOM	2894 2895		TRP I			43.673	43.296	7.204	1.00		В
ATOM	2896	CZ3				41.932	43.452	5.522	1.00	38.70	В
ATOM	2897	CH2	TRP I	3 1	.88	43.249	43.694	5.960	1.00	37.13	В
ATOM	2898	C	TRP I	3 1	88.	38.258	43.455	8.383	1.00		В
MOTA	2899	0	TRP I			37.946	43.240	7.211	1.00		B B
ATOM	2900	N	ARG I			38.442	44.678 45.842	8.864 7.999	1.00		В
ATOM	2901 2902	CA CB	ARG I			38.303 37.731	47.040	8.776	1.00		В
ATOM ATOM	2902	CG	ARG			38.615	47.590	9.893	1.00		В
ATOM	2904	CD	ARG			38.234	47.041	11.270	1.00	59.95	В
ATOM	2905	NB	ARG 1	в	L89	38.639	45.650	11.479		63.62	В
ATOM	2906	CZ	ARG 1			39.903	45.236	11.559		64.33	В
ATOM	2907		ARG			40.899	46.105	11.447		65.45 64.46	B B
ATOM	2908	NH2	ARG :			40.172 39.664	43.951 46.192	11.760 7.412		50.56	В
MOTA MOTA	2909 2910	C O	ARG			40.680	46.119	8.100		50.34	В
ATOM	2911	N	ALA		190	39.684	46.554	6.135		52.30	В
ATOM	2912	CA	ALA			40.933	46.911	5.476		54.16	В
ATOM	2913	CB	ALA :	В:	190	40.846	46.592	3.987		55.33	В
MOTA	2914	С	ALA			41.238	48.392	5.679		55.19	B B
ATOM	2915	0	ALA			40.300	49.147 48.782	6.023 5.481		54.90 56.19	В
MOTA	2916	C	LEU		190	42.408 32.073	1.033	33.225		35.70	č
ATOM ATOM	2917 2918	0	LEU		ī	33.091	1.607	33.619		35.87	С
ATOM	2919	N	LEU		1	29.791	1.906	32.702	1.00	36.17	C
MOTA	2920	CA	LEU	C	1	30.699	1.409	33.777		34.35	C
MOTA	2921	N	GLN		2	32.105	0.072	32.307		34.64	C
MOTA	2922	CA	GLN		2	33.374	-0.359 -0.823	31.737 30.294		33.55	c
MOTA MOTA	2923 2924	0	GLN GLN		2	33.250 32.373	-1.610	29.955		33.68	Ċ
ATOM	2925	N	PRO		3	34.130	-0.329	29.418	1.00	33.74	С
ATOM	2926	CD	PRO		3	35.226	0.632	29.639	1.00	33.81	C
ATOM	2927	CA	PRO	C	3	34.064	-0.742	28.015		34.77	C
MOTA	2928	CB	PRO		3	35.027	0.222	27.329		34.33 34.78	C
MOTA	2929	CG	PRO		3	36.070	0.449 -2.195	28.393 27.890		34.42	c
MOTA	2930	C	PRO		3 3	34.508 35.435	-2.626	28.579		34.76	c
ATOM ATOM	2931 2932	И	PHE		4	33.837		27.024		31.97	C
MOTA	2933	CA			4	34.173	-4.355	26.812		32.26	С
MOTA	2934	СВ			4	32.897		26.632		34.22	c
MOTA	2935	CG			4	32.006				37.02	C
MOTA	2936		1 PHE		4	32.481				38.53 40.29	c
MOTA MOTA	2937 2938		2 PHE 1 PHE		4 4	30.701 31.673				40.80	Ċ
ATOM	2939		2 PHE		4	29.878				41.19	С
ATOM	2940	CZ			4	30.369			1.00	40.74	С
MOTA	2941	C	PHE	C	4	35.052				29.17	C
ATOM	2942	0	PHE		4	34.655				30.93	C
MOTA	2943	N	PRO		5	36.257				26.63 24.97	C
MOTA	2944	CD			5 5	36.936 37.1 68				23.69	Ċ
MOTA MOTA	2945 2946				5	38.527				23.66	С
MOTA	2947				5	38.335			1.00	23.13	C
ATOM	2948		PRO		5	37.043	-6.569			22.95	C
MOTA	2949		PRO		5	36.403				22.96	C
MOTA	2950		GLN		6	37.666				23.53	c
ATOM	2951				6 6	37.659 37.506				20.90	c
MOTA MOTA	2952 2953				6	36.170				21.10	C
ATOM	2954				6	36.074	-6.901	18.557		22.85	C
MOTA	2955		31 GLN		6	36.483	3 -7.760	17.773	1.00	23.94	С

ATOM	2956	NE2	GLN	C	6	35.525	-5.766	18.149	1.00 20.70	C
MOTA	2957	С	GLN	C	6	38.996	-8.637	22.204	1.00 20.71	C
ATOM	2958	0	GLN	C	6	40.046	-8.008	22.105	1.00 19.85	C
ATOM	2959	N	PRO		7	38.974	-9.932	22.548	1.00 21.37	С
					7		-10.710	23.017	1.00 21.21	č
ATOM	2960	CD .	PRO							
MOTA	2961	CA	PRO		7		-10.673	22.790	1.00 21.62	C
ATOM	2962	CB	PRO	C	7	39.783	-11.730	23.795	1.00 21.96	С
ATOM	2963	CG	PRO	C	7	38.416	-12.085	23.297	1.00 20.65	С
ATOM	2964	С	PRO		7	40.741	-11.316	21.511	1.00 24.05	C
					7		-11.577	20.588	1.00 22.84	c
ATOM	2965	0	PRO							Ċ
MOTA	2966	N	GLU		8		-11.550	21.448	1.00 26.22	
ATOM	2967	CA	GLU	C	8	42.631	-12.215	20.292	1.00 27.00	C
ATOM	2968	CB	GLU	C	8	44.038	-11.687	19.988	1.00 27.94	C
ATOM	2969	CG	GLU	C	8	44.803	-12.494	18.915	1.00 28.38	Ç
ATOM	2970	CD	GLU		8	44.043	-12.649	17.589	1.00 31.32	C
							-13.309	17.564	1.00 31.69	C
MOTA	2971		GTA		8					
MOTA	2972	OE2	GLU	С	8		-12.112	16.563	1.00 29.86	C
ATOM	2973	C	GLU	C	8	42.678	-13.691	20. 6 76	1.00 28.48	C
MOTA	2974	0	GLU	С	8	42.937	-14.029	21.829	1.00 28.74	С
ATOM	2975	N	LEU		9	42.407	-14.571	19.721	1.00 30.08	С
					9		-15.998	20.002	1.00 31.21	C
ATOM	2976	CA	LEU							Č
ATOM	2977	CB	LEU		9		-16.688	19.183	1.00 32.12	
MOTA	2978	CG	LEU	С	9		-16.072	19.302	1.00 33.78	C
ATOM	2979	CD1	LEU	C	9	38.941	-16.866	18.457	1.00 35.00	С
ATOM	2980	CD2	LEU	С	9	39,481	-16.061	20.761	1.00 35.59	C
	2981	C	LEU		9		-16.641	19.712	1.00 31.83	c
ATOM								18.658	1.00 30.94	Č
MOTA	2982	0	LEU		9		-16.415			č
ATOM	2983	N	PRO	С	10		-17.442	20.657	1.00 33.31	
ATOM	2984	œ	PRO	C	10	43.774	-17.661	22.032	1.00 33.12	С
ATOM	2985	CA	PRO	C	10	45.545	-18.097	20.439	1.00 36.08	C
ATOM	2986	CB	PRO		10	45.926	-18.590	21.836	1.00 36.62	C
		CG	PRO		10		-18.846	22.476	1.00 35.26	C
ATOM	2987								1.00 37.51	č
MOTA	2988	С	PRO		10		-19.229	19.430		
MOTA	2989	0	PRO	С	10		-20.030	19.491	1.00 39.49	C
ATOM	2990	N	TYR	C	11	46.365	-19.269	18.488	1.00 38.68	С
ATOM	2991	CA	TYR	C	11	46.392	-20.305	17.463	1.00 40.24	C
ATOM	2992	C	TYR		11		-20.782	17.290	1.00 42.03	C
			TYR		11		-21.967	17.586	1.00 42.72	C
ATOM	2993	0							1.00 42.75	C
ATOM	2994		TYR		11		-19.949	16.870		
ATOM	2995	CB	VAL	D	2	76.722	40.050	4.030	1.00 35.81	D
MOTA	2996	CG1	VAL	D	2	77.537	40.465	2.823	1.00 36.64	D
ATOM	2997	CG2	VAL	D	2	76.313	38.577	3.893	1.00 37.71	ם
ATOM	2998	C	VAL		2	76.622		6.537	1.00 31.61	D
			VAL		2	75.696		6.653	1.00 31.96	D
MOTA	2999	0							1.00 32.12	D
MOTA	3000	N	VAL		2	78.625		5.418		
ATOM	3001	CA	VAL	D	2	77.560	40.255	5.317	1.00 33.74	D
MOTA	3002	N	ALA	D	3	76.864	41.246	7.441	1.00 29.52	D
ATOM	3003	CA	ALA	Œ	3	76.053	41.379	8.653	1.00 27.92	D
ATOM	3004	СВ	ALA		3	76.480		9.684	1.00 27.11	D
						76.128		9.286	1.00 25.71	D
MOTA	3005	C	ALA		3				1.00 23.11	D
MOTA	3006	0	ALA		3	77.050		9.016		
MOTA	3007	N	ASI	םי	4	75.152		10.137	1.00 24.26	D
MOTA	3008	CA	ASI	D	4	75.109	44.354	10.825	1.00 24.77	ם
MOTA	3009	CB	ASI	םי	4	73.774	44.533	11.555	1.00 25.88	D
MOTA	3010	CG	ASI		4	72.595	44.668	10.611	1.00 26.24	D
						71.449		11.080	1.00 24.74	D
ATOM	3011		LASI		4			9.416	1.00 28.25	D
MOTA	3012		2 ASI		4	72.81				
MOTA	3013	C	ASI		4	76.230		11.857	1.00 25.96	D
MOTA	3014	0	ASI	פי	4	76.882	2 45.437	12.027	1.00 26.40	D
MOTA	3015	N	HIS	D	5	76.440	43.290	12.549	1.00 24.52	D
ATOM	3016	CA	HIS		5	77.469	43.204	13.582	1.00 24.25	Ð
ATOM	3017	CB	HIS		5	76.836		14.972	1.00 23.42	D
								15.231	1.00 26.12	D
ATOM	3018	CG		3 D	5	76.138				D
ATOM	3019		2 HI		5	76.56		15.126	1.00 26.16	
MOTA	3020	ND:	1 HI	S D	5	74.830		15.657	1.00 25.67	D
ATOM	3021	CE:	1 HI	S D	5	74.483	1 45.932	15.799	1.00 26.53	D
ATOM	3022		2 HI		5	75.51		15.484	1.00 25.96	D
ATOM	3023			S D	5	78.24		13.492	1.00 22.88	D
						77.65		13.258	1.00 22.31	D
ATOM	3024			SD	5				1.00 20.27	D
ATOM	3025			L D	6	79.55		13.691		
MOTA	3026			LD	6	80.42		13.657	1.00 19.49	D.
ATOM	3027	CB	VA	ьD	6	81.41		12.486	1.00 20.45	D
ATOM	3028	CG	1 VA	L D	6	82.35	7 39.674	12.564	1.00 19.85	D
ATOM	3029		2 VA		6	80.67		11.161	1.00 25.29	D
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ATOM	3030	C	VAL	D	6	81.223	40.792	14.944	1.00 18.77	D
ATOM	3031	ō	VAL		6	81.767	41.812	15.352	1.00 17.70	D
ATOM	3032	N	ALA		7	81.304	39.626	15.575	1.00 18.23	D
ATOM	3033	CA	ALA		7	82.046	39.489	16.821	1.00 18.01	מ
MOTA	3034	СВ	ALA		7	81.080	39.452	18.006	1.00 17.61	D
ATOM	3035	C	ALA		7	82.899	38.239	16.838	1.00 17.37	D
ATOM	3036	0	ALA	D	7	82.568	37.242	16.208	1.00 19.56	D
ATOM	3037	N	SER		8	84.008	38.306	17.562	1.00 17.07	D
ATOM	3038	CA	SER	D	8	84.892	37.158	17.712	1.00 15.46	D
MOTA	3039	CB	SER		8	86.297	37.455	17.202	1.00 12.56	D
MOTA	3040	OG	SER	D	8	86.324	37.492	15.789	1.00 18.97	D
ATOM	3041	С	SER	D	8	84.932	36.904	19.201	1.00 16.39	D
ATOM	3042	0	SER	D	8	85.613	37.614	19.951	1.00 15.61	D
ATOM	3043	N	TYR	D	9	84.144	35.930	19.637	1.00 17.58	D
MOTA	3044	CA	TYR	D	9	84.096	35.587	21.044	1.00 18.51	D
MOTA	3045	CB	TYR	D	9	82.698	35.133	21.444	1.00 17.92	D
MOTA	3046	CG	TYR	D	9	81.730	36.290	21.362	1.00 17.41	D
MOTA	3047	CD1	TYR	D	9	82.056	37.523	21.928	1.00 16.27	D
MOTA	3048	CB1	TYR	D	9	81.208	38.603	21.840	1.00 15.18	D
MOTA	3049	CD2	TYR	D	9	80.515	36.169	20.701	1.00 17.05	D
MOTA	3050	CE2	TYR	D	9	79.649	37.252	20.608	1.00 18.01	D
MOTA	3051	CZ	TYR	D	9	80.005	38.466	21.181	1.00 16.67	D
MOTA	3052	OH	TYR	D	9	79.157	39.543	21.104	1.00 20.30	D
MOTA	3053	С	TYR	D	9	85.120	34.508	21.115	1.00 19.92	D
ATOM	3054	0	TYR		9	84.856	33.323	21.337	1.00 17.21	D
MOTA	3055	N	GLY		10	86.321	34.989	20.843	1.00 22.61	D
ATOM	3056	CA	GLY		10	87.478	34.160	20.836	1.00 20.96	D
ATOM	3057	С	GLY		10	88.358	34.354	19.624	1.00 18.79	D
ATOM	3058	0	GLY		10	88.170	33.693	18.618	1.00 16.79	D
MOTA	3059	N	VAL		11	89.275	35.307	19.683	1.00 17.75	D
MOTA	3060	CA	VAL		11	90.256	35.394	18.616	1.00 16.92 1.00 17.76	D D
MOTA	3061	CB	VAL		11	90.666	36.829	18.242	1.00 17.76	D
ATOM	3062		VAL		11	91.873	36.778	17.313	1.00 13.40	D
ATOM	3063		VAL		11	89.522	37.544	17.544	1.00 17.46	D
MOTA	3064	C	VAL		11	91.391	34.728	19.395	1.00 17.40	D
ATOM	3065	0	VAL		11	91.865	35.266	20.405 18.973	1.00 17.46	D
ATOM	3066	N	ASN		12	91.773	33.531 32.779	19.644	1.00 18.01	D
ATOM	3067	CA	ASN		12	92.831		19.969	1.00 16.68	D
MOTA	3068	CB	ASN		12	92.339 91.179	31.360 31.356	20.955	1.00 16.27	D
ATOM	3069	CG	ASN		12	91.346	30.989	22.115	1.00 14.97	D
ATOM	3070		ASN		12 12	90.000	31.779	20.497	1.00 14.97	ם
ATOM	3071		ASN		12	94.061	32.699	18.759	1.00 18.74	ס
ATOM	3072	C O	ASN ASN		12	93.963	32.373	17.578	1.00 19.66	D
ATOM ATOM	3073 3074	N	LEU		13	95.221	32.969	19.344	1.00 20.75	D
	3075	CA	LEU		13	96.471	32.949	18.600	1.00 22.59	D
MOTA MOTA	3075	CB	LEU		13	96.841	34.387	18.234	1.00 24.32	D
ATOM	3077	CG	LEU		13	98.215	34.672	17.632	1.00 25.29	D
ATOM	3078		LEU		13	98.355	33.966	16.289	1.00 24.58	D
ATOM	3079	CD2			13	98.380	36.177	17.475	1.00 23.52	D
ATOM	3080	C	LEU		13	97.646	32.290	19.330	1.00 22.44	D
MOTA	3081	ō	LEU		13	97.900	32.578	20.494	1.00 24.67	D
ATOM	3082	N	TYR		14	98.350	31.397	18.641	1.00 23.69	D
ATOM	3083	CA	TYR		14	99.535	30.740	19.196	1.00 25.57	D
ATOM	3084	СВ	TYR		14	99.223	29.360	19.765	1.00 26.53	D
MOTA	3085	CG	TYF		14	100.445	28.712	20.383	1.00 28.87	α
ATOM	3086		LTYF		14	100.872	29.057	21.668	1.00 28.57	a
MOTA	3087		TYF		14	102.032	28.500	22.218	1.00 27.29	D
ATOM	3088		TYF		14	101.209	27.793	19.664	1.00 29.65	D
ATOM	3089		2 TYF		14	102.369	27.235	20.204	1.00 26.94	D
ATOM	3090	CZ	TYF	R D	14	102.773	27.592	21.477	1.00 27.22	D
ATOM	3091	OH	TYF		14	103.914	27.039	22.008	1.00 29.69	D
ATOM	3092	C	TY	Q S	14	100.553	30.574	18.074	1.00 26.73	D
MOTA	3093	0	TY	R D	14	100.210	30.128	16.980	1.00 27.22	D
ATOM	3094	N	GL	D V	15	101.800	30.945	18.338	1.00 26.92	D
MOTA	3095	CA	GLI	d D	15	102.847	30.820	17.332	1.00 27.70	D
MOTA	3096	CB	GFI	N D	15	103.164	32.179	16.710	1.00 27.39	D
ATOM	3097	CG	GL	N D	15	103.534	33.251	17.704	1.00 27.78	D
MOTA	3098			1 D	15	103.806	34.590	17.044	1.00 27.70	D
MOTA	3099		1 GL		15	103.723	35.638	17.685	1.00 31.07	D
MOTA	3100		2 GI		15	104.142	34.562	15.763	1.00 25.83	D
MOTA	3101			N D	15	104.097	30.222	17.952	1.00 28.40	D
ATOM	3102			N D	15	104.368	30.416	19.141	1.00 28.81	D D
MOTA	3103	N	SE	R D	16	104.852	29.488	17.143	1.00 27.95	,

					106 070	20 024	17.611	1.00 28.04	D
ATOM	3104	CA	SER D	16	106.070	28.834	16.534	1.00 25.04	D
MOTA	3105	CB	SER D	16	106.613	27.887		1.00 26.28	D
ATOM	3106	OG	SER D	16	106.879	28.581	15.330	1.00 27.77	D
MOTA	3107	C	SER D	16	107.155	29.824	18.024		D
MOTA	3108	0	SER D	16	107.922	29.558	18.946	1.00 26.81	
MOTA	3109	N	TYR D	17	107.221	30.965	17.351	1.00 29.70	D
MOTA	3110	CA	TYR D	17	108.228	31.953	17.694	1.00 32.41	D
ATOM	3111	CB	TYR D	17	108.248	33.086	16.672	1.00 35.15	D
ATOM	3112	CG	TYR D	17	109.440	33.986	16.864	1.00 40.80	D
ATOM	3113		TYR D	17	110.719	33.556	16.508	1.00 43.28	D
ATOM	3114		TYR D	17	111.836	34.345	16.743	1.00 44.62	D
ATOM	3115		TYR D	17	109.308	35,235	17.460	1.00 40.97	D
	3116	CE2	TYR D	17	110.419	36.032	17.702	1.00 44.83	ם
ATOM				17	111.679	35.580	17.341	1.00 45.74	D
ATOM	3117	CZ	TYR D		112.788	36.353	17.590	1.00 49.39	D
MOTA	3118	OH	TYR D	17			19.084	1.00 33.13	D
ATOM	3119	C	TYR D	17	107.954	32.525		1.00 33.13	Ď
ATOM	3120	0	TYR D	17	106.888	33.092	19.332		D
ATOM	3121	N	GLA D	18	108.930	32.383	19.981	1.00 32.74	
ATOM	3122	CA	GLY D	18	108.780	32.867	21.341	1.00 31.76	D
ATOM	3123	C	GLY D	18	108.958	31.716	22.311	1.00 32.63	D
ATOM	3124	0	GLY D	18	110.005	31.600	22.948	1.00 34.20	D
ATOM	3125	N	PRO D	19	107.946	30.840	22.452	1.00 33.13	D
ATOM	3126	CD	PRO D	19	108.029	29.606	23.256	1.00 31.73	D
ATOM	3127	CA	PRO D	19	106.663	30.906	21.741	1.00 32.71	D
MOTA	3128	CB	PRO D	19	106.115	29.492	21.903	1.00 33.20	D
ATOM	3129	CG	PRO D	19	. 106.591	29.128	23.280	1.00 31.76	Q
	3130	C	PRO D	19	105.768	31.948	22.406	1.00 32.52	D
ATOM	3131	ō	PRO D	19	105.970	32.282	23.568	1.00 33.11	D
MOTA		N	SER D	20	104.786	32.463	21.676	1.00 31.92	D
ATOM	3132		SER D	20	103.886	33.455	22,246	1.00 30.99	D
ATOM	3133	CA		20	104.287	34.867	21.795	1.00 30.92	D
ATOM	3134	СВ	SER D		104.263	34.988	20.381	1.00 33.16	D
ATOM	3135	OG	SER D	20	102.441	33.172	21.852	1.00 30.01	D
ATOM	3136	C	SER D	20		32.428	20.902	1.00 29.42	D
MOTA	3137	0	SER D	20	102.179	33.763	22.598	1.00 27.60	D
ATOM	3138	N	GLY D	21	101.512		22.318	1.00 25.70	D
MOTA	3139	CA	GLY D	21	100.101	33.580	22.632	1.00 24.66	Đ
MOTA	3140	С	GLY D	21	99.309	34.836		1.00 23.84	D
ATOM	3141	0	GLY D	21	99.848	35.798	23.187	1.00 22.55	D
MOTA	3142	N	GLN D	22	98.030	34.834	22.268	1.00 20.16	D
ATOM	3143	CA	GTM D		97.149	35.974	22.527	1.00 20.18	D
MOTA	3144	СВ	GTM D		97.301	37.049	21.445		Ď
MOTA	3145	CG	GLN D		96.416	38.284	21.672	1.00 18.60	D
ATOM	3146	CD	GLN D		96.513	39.327	20.562	1.00 18.36	Ď
MOTA	3147		L GLN D		97.379	40.207	20.587	1.00 19.82	D
ATOM	3148	NE:	2 GLN D		95.617	39.232	19.582	1.00 17.69	
ATOM	3149	C	GLN D		95.699	35.517	22.561	1.00 18.61	D
MOTA	3150	0	GLN D	22	95.301	34.638	21.790	1.00 17.26	D
MOTA	3151	N	TYR D	23	94.926	36.097	23.475	1.00 16.42	D
ATOM	3152	CA	TYR D	23	93.507	35.785	23.592	1.00 16.21	D
ATOM	3153	CB	TYR I	23	93.212	34.839	24.762	1.00 14.97	D
MOTA	3154	CG	TYR I	23	91.750	34.438	24.798	1.00 14.24	D
ATOM	3155				91.309	33.318	24.109	1.00 14.49	Ð
ATOM	3156		1 TYR I		89.969	33.004	24.029	1.00 14.23	D
MOTA	3157		2 TYR I		90.795		25.421	1.00 13.21	D
	3158		2 TYR I		89.443			1.00 13.0B	D
MOTA					89.039			1.00 12.88	D
MOTA	3159				87.710				Œ
MOTA	3160				92.751				D
MOTA	3161		TYR I		93.014				D
MOTA	3162		TYR I		91.811				D
MOTA	3163		THR I						Œ
MOTA	3164				91.026				D
MOTA	3165				91.606				D
MOTA	3166		1 THR		91.682				D
ATOM	3167	, CG	2 THR		92.992				ď
MOTA	3168	C	THR :		89.604				D
ATOM	3169		THR 1		89.306				Ď
ATOM	3170		HIS		88.726				D
MOTA	3171				87.360				D
MOTA	3172				86.326				ם
ATOM	3173				86.053				ם
MOTA	3174		2 HIS		86.81				D
MOTA	3175	NI C	O1 HIS	D 25	84.87				
ATOM	3176		Z1 HIS	D 25	84.92				D D
ATOM	3177		E2 HIS	D 25	86.08	35.59	24.289	1.00 13.67	J

ATOM	3178	C	HIS	D	25	87.158	40.495	21.436	1.00 13.30	D
ATOM	3179	ō	HIS		25	87.573	41.563	21.859	1.00 13.77	D
					26				1.00 15.40	ď
ATOM	3180	N	GLU			86.544	40.376	20.271		
ATOM	3181	CA	GLU		26	86.318	41.540	19.434	1.00 16.53	D
ATOM	3182	CB	GLU		26	87.109	41.396	18.133	1.00 14.47	D
MOTA	3183	CG	GLU	D	26	88.627	41.460	18.277	1.00 14.81	D
ATOM	3184	CD	GLU	D	26	89.341	41.205	16.947	1.00 19.22	D
ATOM	3185	OE1	GLU	D	26	88.726	41.429	15.884	1.00 22.84	D
ATOM	3186	OE2	GLU	D	26	90.512	40.792	16.953	1.00 17.41	D
ATOM	3187	C	GLU		26	84.841	41.721	19.111	1.00 17.28	D
ATOM	3188	ō	GLU		26	84.073	40.760	19.100	1.00 16.62	D
		N	PHE		27	84.455	42.971	18.879	1.00 19.63	D
ATOM	3189									
ATOM	3190	CA	PHE		27	83.092	43.313	18.494	1.00 19.71	D
ATOM	3191	CB	PHE		27	82.231	43.722	19.684	1.00 21.05	D
ATOM	3192	CG	PHE		27	80.758	43.816	19.348	1.00 24.29	D
ATOM	3193		PHE		27	79.971	42.668	19.278	1.00 23.22	D
ATOM	3194	CD2	PHE	D	27	80.169	45.047	19.073	1.00 22.47	D
ATOM	3195	CE1	PHE	D	27	78.617	42.744	18.940	1.00 24.89	D
ATOM	3196	CE2	PHE	D	27	78.818	45.132	18.733	1.00 24.72	D
ATOM	3197	CZ	PHE	D	27	78.041	43.980	18.667	1.00 22.80	D
MOTA	3198	C	PHE		27	83.182	44.482	17.532	1.00 18.41	D
ATOM	3199	ō	PHE		27	83.700	45.545	17.879	1.00 19.21	D
			ASP		28		44.272	16.321	1.00 18.46	ם
MOTA	3200	N				82.680				
ATOM	3201	CA	ASP		28	82.700	45.284	15.272	1.00 18.63	D
MOTA	3202	СВ	ASP		28	81.702	46.404	15.568	1.00 19.29	D
MOTA	3203	CG	ASP		28	80.268	45.981	15.305	1.00 22.52	D
ATOM	3204	OD1	ASP	D	28	80.076	44.885	14.738	1.00 23.13	D
MOTA	3205	OD2	ASP	D	28	79.333	46.736	15.651	1.00 24.61	D
ATOM	3206	С	ASP	D	28	84.075	45.865	15.037	1.00 17.83	D
ATOM	3207	0	ASP	D	28	84.225	47.069	14.860	1.00 20.60	D
ATOM	3208	N	GLY	D	29	85.079	44.997	15.042	1.00 18.44	D
ATOM	3209	CA	GLY		29	86.439	45.431	14.788	1.00 19.49	D
ATOM	3210	C	GLY		29	87.218	46.011	15.949	1.00 18.93	D
							46.359	15.784	1.00 19.51	D
ATOM	3211	0	GLY		29	88.382				D
ATOM	3212	N	ASP		30	86.595	46.122	17.117	1.00 17.91	
MOTA	3213	CA	asp		30	87.279	46.667	18.288	1.00 17.21	ם
MOTA	3214	CB	ASP	D	30	86.499	47.858	18.831	1.00 15.85	D
MOTA	3215	CG	ASP	D	30	86.594	49.060	17.924	1.00 18.96	D
MOTA	3216	OD1	ASP	D	30	87.731	49.515	17.668	1.00 18.56	D
MOTA	3217	OD2	ASP	D	30	85.541	49.544	17.466	1.00 19.00	D
ATOM	3218	С	ASP	D	30	87.491	45.629	19.389	1.00 17.20	D
ATOM	3219	ō	ASP		30	86.651	44.763	19.621	1.00 15.68	D
ATOM	3220	N	GLU		31	88.629	45.739	20.062	1.00 18.79	D
		CA	GLU		31	89.015	44.829	21.131	1.00 17.52	D
ATOM	3221		GTA			90.531	44.947	21.363	1.00 19.03	D
ATOM	3222	CB			31				1.00 22.08	Ď
ATOM	3223	CG	GLU		31	91.074	44.215	22.579		
MOTA	3224	Э	GLU		31	92.596	44.254	22.653	1.00 25.29	D
ATOM	3225		GLU		31	93.198	45.159	22.041	1.00 26.54	D
MOTA	3226	OE2	GLU	D	31	93.193	43.387	23.331	1.00 25.19	D
ATOM	3227	C	GLU	D	31	88.248	45.109	22.421	1.00 17.80	D
ATOM	3228	0	GLU	D	31	88.360	46.195	23.004	1.00 16.81	Ø
ATOM	3229	N	GLN	D	32	87.478	44.118	22.862	1.00 15.25	Ø
ATOM	3230	CA	GLN	D	32	86.685	44.230	24.085	1.00 15.53	D
ATOM	3231	СВ	GLN		32	85.502	43.260	24.044	1.00 12.86	ם
ATOM	3232	CG	GLN		32	84.391	43.680	23.101	1.00 13.72	D
			GLN		32	83.233	42.708	23.111	1.00 16.53	D
ATOM	3233	CD				83.407	41.526	22.838	1.00 20.27	D
ATOM	3234		GLN		32					D
MOTA	3235		GLN		32	82.044	43.203	23.423	1.00 17.48	
MOTA	3236	C	GLN		32	87.528	43.956	25.329	1.00 16.00	D
ATOM .	3237	0	GLN	D	32	87.356	44.603	26.366	1.00 15.18	Ø
MOTA	3238	N	PHE	D	33	88.423	42.981	25.222	1.00 16.17	ם
MOTA	3239	CA	PHE	D	33	89.315	42.638	26.321	1.00 15.74	D
ATOM	3240	CB	PHE	D	33	88.520	42.083	27.515	1.00 15.40	D
ATOM	3241	CG	PHE	D	33	87.969	40.693	27.307	1.00 15.83	D
ATOM	3242		PHE		33	88.781	39.572	27.480	1.00 16.23	D
ATOM	3243		PHE		33	86.625	40.503	26.977	1.00 17.27	D
MOTA	3244		PHE		33	88.262	38.282	27.332	1.00 15.79	ם
						86.088	39.218	26.827	1.00 15.20	. D
ATOM	3245		PHE		33			27.006	1.00 17.77	ā
ATOM	3246	cz	PHE		33	86.909	38.108		1.00 17.77	D
MOTA	3247	C	PHE		33	90.330	41.614	25.860		
ATOM	3248	0	PHE		33	90.157	40.979	24.825	1.00 15.16	D
ATOM	3249	N	TYR		34	91.405	41.476	26.620	1.00 15.54	D
MOTA	3250	CA	TYR		34	92.414	40.480	26.314	1.00 16.00	D
MOTA	3251	CB	TYR	D	34	93.649	41.124	25.670	1.00 17.46	D

						04 500	41 070	25 500	1 00 00 00	D
ATOM	3252	CG	TYR I		4	94.508	41.970	26.588	1.00 20.90	
ATOM	3253	CD1	TYR I		4	95.488	41.390	27.391	1.00 21.91	D
ATOM	3254	CE1	TYR I) 3	4	96.295	42.174	28.221	1.00 24.17	D
MOTA	3255	CD2	TYR I) 3	14	94.351	43.354	26.638	1.00 20.26	D
ATOM	3256	CE2	TYR I	3	34	95.147	44.141	27.463	1.00 24.97	D
ATOM	3257	CZ	TYR I	3	34	96.117	43.546	28.251	1.00 23.87	D
MOTA	3258	OH	TYR I		34	96.904	44.326	29.065	1.00 26.29	D
					34	92.766	39.836	27.642	1.00 16.56	D
MOTA	3259	C	TYR I							D
MOTA	3260	0	TYR I		34	92.476	40.386	28.699	1.00 15.36	
ATOM	3261	N	VAL 1	3	35	93.354	38.653	27.586	1.00 18.29	D
MOTA	3262	CA	VAL 1	D 3	35	93.768	37.971	28.795	1.00 19.11	D
ATOM	3263	CB	VAL 1	D 3	35	93.257	36.514	28.842	1.00 17.61	D
ATOM	3264		VAL I		35	93.910	35.780	29.992	1.00 17.99	D
ATOM	3265		VAL I		35	91.744	36.493	29.003	1.00 17.82	D
		C	VAL		35	95.290	37.950	28.813	1.00 19.96	D
ATOM	3266					95.914	37.492	27.866	1.00 17.73	D
ATOM	3267	0	VAL I		35					D
MOTA	3268	N	ASP 1		36	95.883	38.473	29.880	1.00 22.63	
MOTA	3269	CA	ASP I	D 3	36	97.333	38.456	30.005	1.00 24.79	D
ATOM	3270	CB	ASP :	D 3	36	97.795	39.409	31.106	1.00 26.41	ָ ס
ATOM	3271	CG	ASP I	D ,3	36	99,298	39.574	31.131	1.00 30.12	D
ATOM	3272	OD1	ASP I	D 3	36	100.002	38.547	31.252	1.00 32.04	D
ATOM	3273		ASP 1		36	99.776	40.726	31.028	1.00 32.20	D
ATOM	3274	c	ASP		36	97.650	37.011	30.389	1.00 25.23	D
			ASP		36	97.349	36.575	31.502	1.00 25.21	D
MOTA	3275	0							1.00 23.64	D
MOTA	3276	N	PEO :		37	98.236	36.272	29.455		
ATOM	3277	CA	LEU :		37	98.549	34.870	29.676	1.00 25.25	D
ATOM	3278	CB	LEU	D :	37	98.992	34.232	28.355	1.00 21.08	D
ATOM	3279	CG	TEO :	D :	37	97.955	34.360	27.225	1.00 20.24	D
ATOM	3280	CD1	LEU	D :	37	98.568	33.934	25.899	1.00 17.23	D
ATOM	3281	CD2	LEU	D :	37	96.730	33.516	27.541	1.00 19.11	D
ATOM	3282	c	LEU		37	99.590	34.626	30.770	1.00 27.73	D
	3283	ō	LEU		37	99.464	33.682	31.554	1.00 27.92	D
ATOM							35.474	30.837	1.00 29.31	D
MOTA	3284	N	GLY		38	100.608				Ď
ATOM	3285	CA	GLA		38	101.629	35.292	31.851	1.00 30.44	
MOTA	3286	С	GLY	D :	38	101.141	35.640	33.242	1.00 32.52	D
MOTA	3287	0	GLY	D :	38	101.502	34.986	34.220	1.00 34.37	D
MOTA	3288	N	ARG	D :	39	100.309	36.669	33.335	1.00 35.10	D
ATOM	3289	CA	ARG	D :	39	99.786	37.103	34.623	1.00 36.92	D
ATOM	3290	СВ	ARG		39	99.693	38.632	34.653	1.00 39.96	D
		CG	ARG		39	101.011	39.318	34.301	1.00 44.57	D
ATOM	3291					101.006	40.798	34.667	1.00 49.71	D
MOTA	3292	CD	ARG		39				1.00 53.08	D
MOTA	3293	NE	ARG		39	102.240	41.484	34.270		D
ATOM	3294	\mathbf{cz}	ARG		39	103.460	41.164	34.698	1.00 55.33	
ATOM	3295	NH1	ARG	D	39	103.635	40.158	35.546	1.00 56.98	D
MOTA	3296	NH2	ARG	D	39	104.512	41.859	34.282	1.00 56.80	D
ATOM	3297	С	ARG	D	39	98.429	36.476	34.924	1.00 35.86	D
ATOM	3298	o	ARG		39	97.886	36.630	36.022	1.00 35.27	D
ATOM	3299	N	LYS		40	97.893	35.757	33.944	1.00 34.51	D
			LYS		40	96.602	35.095	34.090	1.00 33.49	D
MOTA	3300	CA				96.714	33.939	35.088	1.00 34.77	D
MOTA	3301	CB	LYS		40			35.133	1.00 41.38	Ď
ATOM	3302	CG	LYS		40	95.482	33.040			D
ATOM	3303	CD	LYS		40	95.703	31.839	36.046	1.00 45.02	
MOTA	3304	CE	LYS	D	40	94.443	31.001	36.185	1.00 46.54	D
ATOM	3305	NZ	LYS	D	40	94.652	29.853	37.112	1.00 48.98	D
MOTA	3306	C	LYS	D	40	95.511	36.064	34.542	1.00 30.95	D
ATOM	3307	0	LYS	D	40	94.780	35.794	35.492	1.00 28.23	ם
ATOM	3308	N	GLU		41	95.401	37.197	33.858	1.00 30.54	α
ATOM	3309	CA	GLU		41	94.384	38.175	34.210	1.00 30.41	D
			GLU		41	94.980	39.302	35.078	1.00 34.10	D
MOTA	3310	CB					40.034	34.488	1.00 41.52	D
ATOM	3311	CG	GLU		41	96.180			1.00 45.72	D
MOTA	3312	CD	GLU		41	96.834	40.997	35.482		
MOTA	3313	OE:	l GLT	D	41	97.826	41.665	35.108	1.00 48.68	D
MOTA	3314	OE:	2 GLU	D	41	96.362	41.086	36.638	1.00 47.60	D
MOTA	3315	C	GLU	D	41	93.651	38.766	33.014	1.00 28.03	D
MOTA	3316	o	GLU		41	94.220	38.981	31.940	1.00 25.49	D
ATOM	3317	N	THR		42	92.364	39.006		1.00 25.48	D
		CA	THR		42	91.488	39.582		1.00 23.42	D
MOTA	3318				42	90.035	39.187		1.00 22.07	D
ATOM	3319	CB	THR						1.00 18.54	D
MOTA	3320		1 THR		42	89.927				D
ATOM	3321		2 THR		42	89.087				D
MOTA	3322	C	THR		42	91.615			1.00 22.29	
ATOM	3323	0	THR	D	42	91.492			1.00 21.54	D
ATOM	3324		VAL	D	43	91.874	41.736			D
ATOM	3325				43	92.004	43.183	31.136	1.00 19.88	D

1 mov	2226	an	VAL	ъ.	43	93.428	43.584	30.697	1.00 21.56	D
MOTA	3326	CB				93.420	45.091	30.828	1.00 20.99	D
ATOM	3327		VAL		43			31.539	1.00 19.79	Ď
ATOM	3328		VAL		43	94.456	42.827	30.164	1.00 20.50	Ď
MOTA	3329	С	VAL		43	90.968	43.744			D
MOTA	3330	0	VAL		43	91.045	43.513	28.959	1.00 19.49	
MOTA	3331	N	TRP		44	89.987	44.466	30.690	1.00 21.49	D
MOTA	3332	CA	TRP		44	88.946	45.028	29.836	1.00 22.88	D
MOTA	3333	CB	TRP	D	44	87.685	45.326	30.649	1.00 21.57	D
ATOM	3334	CG	TRP	D	44	87.167	44.129	31.372	1.00 21.99	D
ATOM	3335	CD2	TRP	D	44	86.280	43.125	30.854	1.00 22.20	D
ATOM	3336	CE2	TRP	D	44	86.119	42.150	31.862	1.00 22.19	D
ATOM	3337	CE3	TRP	D	44	85.611	42.951	29.634	1.00 20.96	D
ATOM	3338	CD1	TRP	D	44	87.492	43.736	32.633	1.00 23.17	D
ATOM	3339	NE1	TRP	D	44	86.868	42.548	32.937	1.00 23.70	D
ATOM	3340		TRP		44	85.311	41.016	31.693	1.00 24.30	D
ATOM	3341	CZ3	TRP		44	84.807	41.824	29.461	1.00 22.81	D
ATOM	3342	-	TRP		44	84.666	40.870	30.487	1.00 24.05	D
ATOM	3343	C	TRP		44	89.425	46.291	29.143	1.00 23.92	D
ATOM	3344	ō	TRP		44	90.081	47.131	29.759	1.00 24.50	D
ATOM	3345	N	CYS		45	89.098	46.417	27.859	1.00 24.24	D
		CA	CYS		45	89.498	47.580	27.069	1.00 26.23	D
MOTA	3346		CYS		45	89.951	47.141	25.672	1.00 25.96	D
ATOM	3347	CB			45	91.422	46.098	25.665	1.00 25.42	D
ATOM	3348	SG	CYS				48.608	26.950	1.00 27.07	D
MOTA	3349	C	CYS		45	88.377	49.749	26.549	1.00 28.23	D
ATOM	3350	0	CYS		45	88.612			1.00 27.18	D
MOTA	3351	N	LEU		46	87.157	48.193	27.273	1.00 27.16	D
MOTA	3352	CA	LEU		46	86.002	49.087	27.232		D
MOTA	3353	CB	LEU		46	84.907	48.525	26.320	1.00 27.82	
ATOM	3354	CG	LEU		46	84.142	49.460	25.372	1.00 30.22	D C
MOTA	3355	CDI	LEU	D	46	82.792	48.827	25.040	1.00 29.72	D
MOTA	3356	CD2	LEU	D	46	83.928	50.827	25.994	1.00 31.10	D
ATOM	3357	C	LEU	D	46	85.504	49.138	28.675	1.00 28.73	Ð
MOTA	3358	0	LEU	D	46	85.049	48.133	29.216	1.00 28.92	D
MOTA	3359	N	PRO	D	47	85.601	50.309	29.318	1.00 29.35	D
ATOM	3360	CD	PRO	D	47	86.116	51.554	28.717	1.00 28.33	D
ATOM	3361	CA	PRO	D	47	85.182	50.533	30.709	1.00 29.01	D
ATOM	3362	CB	PRO	D	47	B5.139	52.051	30.806	1.00 29.32	D
ATOM	3363	CG	PRO	Q (47	86.307	52.447	29.929	1.00 30.61	D
ATOM	3364	С	PRO		47	83.879	49.875	31.169	1.00 28.51	D
ATOM	3365	o	PRO		47	83.867	49.151	32.163	1.00 28.22	D
ATOM	3366	N	VAI		48	82.784	50.126	30.458	1.00 28.05	D
MOTA	3367	CA	VAI		48	81.492	49.545	30.826	1.00 27.41	D
MOTA	3368	CB	VAI		48	80.406	49.918	29.810	1.00 26.31	D
	3369		. VAI		48	79.955	51.345	30.027	1.00 30.25	D
ATOM			VAI		48	80.949	49.744	28.398	1.00 26.11	D
ATOM	3370			פנ	48	81.490	48.022	30.961	1.00 26.77	D
ATOM	3371	C		L D	48	80.622	47.462	31.627	1.00 27.43	D
ATOM	3372	0				82.449	47.353	30.332	1.00 25.75	D
MOTA	3373	N		ם ע			45.898	30.395	1.00 27.21	D
ATOM	3374	CA		J D		82.517		29.153	1.00 27.47	ם
MOTA	3375	CB		U D		83.237	45.354	27.944	1.00 29.74	D
MOTA	3376	CG		ם ס		82.405	44.886		1.00 29.28	D
MOTA	3377		LE			81.361	45.898	27.578	1.00 29.72	D
MOTA	3378	-	FE			83.329	44.627	26.753	1.00 27.86	D
MOTA	3379	С		U D		83.185	45.374	31.674		
MOTA	3380	0		U D		83.246	44.163	31.900	1.00 25.45	Q Q
ATOM	3381	N		G D		83.680	46.283	32.508	1.00 29.82	D
ATOM	3382	CA	AR	G D	50	84.319	45.892	33.768	1.00 32.18	D
MOTA	3383	CB	AR	G D	50	84.900	47.105	34.509	1.00 35.49	D
ATOM	3384	CG	AR	G D	50	86.010	47.890	33.824	1.00 40.53	D
MOTA	3385	CD	AR	G D	50	86.524	48.968	34.786	1.00 42.89	D
MOTA	3386	NE	AR	G E	50	87.297	50.017	34.125	1.00 46.26	D
ATOM	3387	CZ	AR	GI	50	88.484	49.836	33.555	1.00 46.43	D
MOTA	3388		1 AR	G E	50	89.049	48.636	33.564	1.00 46.42	D
MOTA	3389		2 AR			89.100	50.857	32.968	1.00 43.78	D
ATOM	3390			GI		83.283	45.247	34.690		D
MOTA	3391			G I		83.631	44.577	35.664	1.00 31.56	D
ATOM	3392			NI		82.009	_		1.00 30.22	D
ATOM	3393			NI		80.942				D
	3394			NI		79.610				D
ATOM				N I		79.194				D
MOTA	3395			N I		77.888				D
MOTA	3396		1 GI			76.835				D
ATOM	3397					77.951				D
MOTA	3398		2 GI			80.830				D
MOTA	3399	C	GL	N I	J 21	00.030				_

		_	a		00 203	42.721	35.911	1.00 29.09	D
ATOM	3400	0	GLN D		80.291 81.342	42.899	33.935	1.00 28.19	D
MOTA	3401	N	PHE D		81.300	41.468	33.676	1.00 26.27	D
ATOM	3402	CA	DHE D		81.218	41.188	32.178	1.00 25.00	D
ATOM	3403	CB	PHE D		80.030	41.801	31.513	1.00 23.07	ם
MOTA	3404	CG	PHE D		78.744	41.569	31.999	1.00 22.75	D
MOTA MOTA	3405		PHE D		80.188	42.594	30.380	1.00 23.46	D
ATOM	3406 3407		PHE D		77.627	42.122	31.364	1.00 21.26	D
ATOM	3408		PHE D		79.079	43.151	29.735	1.00 21.92	D
ATOM	3409	CZ	PHE D		77.799	42.913	30.231	1.00 21.69	D
ATOM	3410	C	PHE D		82.547	40.797	34.217	1.00 27.11	D
ATOM	3411	ō	PHE D		83.477	41.461	34.669	1.00 27.64	D
ATOM	3412	N	ARG D		82.556	39.471	34.152	1.00 27.25	D
ATOM	3413	CA	ARG D		83.683	38.672	34.609	1.00 28.31	D
ATOM	3414	СВ	ARG D		83.347	37.976	35.939	1.00 32.75	D
MOTA	3415	CG	ARG D		83.263	38.921	37.143	1.00 40.59	D
MOTA	3416	CD	ARG D	53	82.418	38.325	38.269	1.00 45.99	D
ATOM	3417	NE	ARG D	53	81.007	38.229	37.892	1.00 52.14	D
ATOM	3418	CZ	ARG I	53	80.172	39.265	37.808	1.00 53.70	D
MOTA	3419	NHl	ARG I	53	80.597	40.493	38.080	1.00 53.85	D
MOTA	3420	NH2	ARG I	53	78.910	39.071	37.440	1.00 54.61	D
ATOM	3421	C	ARG I		84.007	37.624	33.548	1.00 25.73	D
MOTA	3422	0	ARG I		83.120	37.103	32.875	1.00 23.84	D
MOTA	3423	N	PHE I		85.290	37.335	33.387	1.00 23.47	D
MOTA	3424	CA	PHE I		85.716	36.336	32.425	1.00 19.92	D
MOTA	3425	CB	PHE I		86.159	36.980	31.113	1.00 15.46	D
MOTA	3426	CG	PHE I		86.346	35.994	30.007	1.00 17.29 1.00 15.32	D D
MOTA	3427		PHE I		85.249	35.506	29.303 29.701	1.00 15.32	D
ATOM	3428		PHE I		87.615	35.503	28.309	1.00 16.04	D
MOTA	3429		PHE I		85.415 87.788	34.539 34.535	28.709	1.00 13.99	D
ATOM	3430	CE2	PHE I		86.688	34.055	28.014	1.00 14.35	D
ATOM	3431 3432	C	PHE I		86.879	35.598	33.055	1.00 18.63	D
MOTA	3433	0	PHE I		87.922	36.188	33.329	1.00 19.50	D
MOTA MOTA	3434	N	ASP I		86.676	34.312	33.309	1.00 19.05	D
ATOM	3435	CA	ASP I		87.689	33.466	33.921	1.00 19.33	D
MOTA	3436	CB	ASP I		87.084	32.100	34.237	1.00 21.38	D
MOTA	3437	CG	ASP I		88.090	31.138	34.832	1.00 24.95	D
ATOM	3438		ASP I		89.264	31.528	35.021	1.00 27.01	D
ATOM	3439		ASP I		87.703	29.985	35.112	1.00 27.48	D
ATOM	3440	C	ASP I		88.863	33.323	32.955	1.00 19.84	D
ATOM	3441	0	ASP I	D 55	88.741	32.691	31.904	1.00 18.07	Ø
ATOM	3442	N	PRO 1	D 56	90.024	33.909	33.311	1.00 19.36	D
MOTA	3443	CD	PRO 1	D 56	90.285	34.584	34.593	1.00 16.09	D
MOTA	3444	CA	PRO 1	D 56	91.240	33.867	32.486	1.00 18.34	D
MOTA	3445	CB	PRO 1		92.228	34.729	33.278	1.00 19.78	D
MOTA	3446	CG	PRO :	D 56	91.792	34.517	34.692	1.00 18.66	מ
MOTA	3447	C	PRO 1		91.770	32.468	32.206	1.00 18.30	D
MOTA	3448	0	PRO		92.583	32.277	31.299	1.00 17.41	ď
MOTA	3449	N	GLN		91.304	31.489	32.977	1.00 18.31	D D
MOTA	3450	CA	GLN		91.744	30.114	32.781	1.00 18.39	D
MOTA	3451	CB	GLN		91.314	29.233	33.963 33.856	1.00 19.94 1.00 18.50	D
MOTA	3452	CG	GLN		91.738	27.773 27.603	33.765	1.00 23.86	D
ATOM	3453	CD	GLN		93.252 94.000	28.110	34.612	1.00 23.68	D
ATOM	3454	NE2	GLN		93.709	26.885	32.739	1.00 19.56	D
ATOM ATOM	3455 3456	C	GLN		91.174	29.555	31.480	1.00 20.01	D
ATOM	3457	ō	GLN		91.733	28.618	30.903	1.00 19.26	D
ATOM	3458	N	PHE		90.059	30.113	31.016	1.00 19.19	D
MOTA	3459	CA	PHE		89.490	29.629	29.765	1.00 20.37	D
MOTA	3460	СВ	PHE		88.178	30.347	29.427	1.00 18.69	D
ATOM	3461	CG	PHE		87.587		28.114	1.00 20.67	D
ATOM	3462		L PHE		88.040	30.456	26.912	1.00 19.84	D
MOTA	3463		2 PHE		86.640	28.891	28.070	1.00 19.87	D
ATOM	3464	CE:	1 PHE	D 58	87.562	29.984	25.682	1.00 19.25	Ø
ATOM	3465				86.156	28.411	26.844	1.00 20.67	D
ATOM	3466		PHE	D 58	86.623		25.652		D
ATOM	3467		PHE	D 58			28.659		D
MOTA	3468		PHE				27.790		D
ATOM	3469		ALA			•			D
MOTA	3470	CA							D
ATOM	3471	CB							D
ATOM	3472		ALA						D
MOTA	3473	0	ALA	D 59	93.877	30.151	26.796	1.00 22.54	D

				_			20 400	20 020	1.00 21.24	D
MOTA	3474	N	LEU		60	93.890	30.409	29.030		
MOTA	3475	CA	TEA	D	60	95.101	29.601	29.188	1.00 22.31	D
ATOM	3476	CB	LEU	D	60	95.501	29.474	30.663	1.00 22.79	D
ATOM	3477	CG	LEU	D	60	96.063	30.698	31.393	1.00 25.87	Œ
ATOM	3478	CD1			60	96.455	30.303	32.805	1.00 28.75	Ø
		CD2			60	97.270	31.223	30.670	1.00 28.42	D
MOTA	3479						28.207	28.617	1.00 21.85	D
MOTA	3480	C	LEU		60	94.891				D
MOTA	3481	0	LEU		60	95.731	27.691	27.875	1.00 22.48	
ATOM	3482	N	THR	D	61	93.763	27.600	28.966	1.00 19.32	D
MOTA	3483	CA	THR	D	61	93.457	26.259	28.489	1.00 20.67	D
ATOM	3484	CB	THR	D	61	92.175	25.721	29.158	1.00 20.04	D
ATOM	3485		THR		61	92.419	25.539	30.558	1.00 23.09	D
			THR		61	91.759	24.393	28.546	1.00 21.15	D
ATOM	3486						26.240	26.974	1.00 19.50	D
ATOM	3487	C	THR		61	93.283				D
ATOM	3488	0	THR	D	61	93.805	25.363	26.288	1.00 18.76	
MOTA	3489	N	ASN	D	62	92.565	27.229	26.456	1.00 19.66	D
ATOM	3490	CA	ASN	D	62	92.310	27.300	25.032	1.00 19.00	ם
ATOM	3491	CB	ASN	D	62	91.356	28.453	24.729	1.00 18.52	ם
ATOM	3492	CG	ASN		62	90.262	28.052	23.760	1.00 20.31	D
			ASN		62	89.726	26.942	23.833	1.00 19.27	D
MOTA	3493						28.952	22.854	1.00 22.25	D
ATOM	3494		ASN		62	89.917				ם
ATOM	3495	С	ASN		62	93.599	27.445	24.244	1.00 19.63	
MOTA	3496	0	ASN	D	62	93.774	26.788	23.221	1.00 21.16	D
MOTA	3497	N	ILE	D	63	94.509	28.290	24.724	1.00 19.68	D
ATOM	3498	CA	ILE	D	63	95.779	28.481	24.033	1.00 18.76	D
ATOM	3499	СВ	ILE		63	96.587	29.660	24.645	1.00 18.72	D
					63	97.946	29.780	23.966	1.00 17.99	D
MOTA	3500	CG2				95.813	30.968	24.471	1.00 17.09	D
ATOM	3501		ILE		63				1.00 17.47	D
MOTA	3502	CD1	ILE		63	95.507	31.313	23.017		
ATOM	3503	C	ILE	D	63	96.613	27.195	24.094	1.00 18.86	D
MOTA	3504	0	ILE	D	63	97.354	26.885	23.164	1.00 20.67	D
ATOM	3505	N	ALF	D	64	96.497	26.448	25.188	1.00 18.22	D
	3506	CA	ALA		64	97.244	25.193	25.316	1.00 20.33	D
ATOM					64	97.039	24.574	26.708	1.00 17.30	D
MOTA	3507	СВ	ALA				24.232	24.233	1.00 21.38	D
MOTA	3508	C	AL/		64	96.756				D
MOTA	3509	0	ALA	7 D	64	97.536	23.459	23.677	1.00 23.44	
MOTA	3510	N	VAI	םי	65	95.459	24.290	23.940	1.00 21.97	D
ATOM	3511	CA	VAI	םי	65	94.872	23.444	22.910	1.00 22.59	D
ATOM	3512	CB	VAI	םי	65	93.324	23.570	22.890	1.00 22.30	D
	3513		. VAI		65	92.744	22.781	21.728	1.00 17.73	D
ATOM					65	92.747	23.053	24.204	1.00 19.10	D
ATOM	3514	CG2						21.541	1.00 23.65	D
MOTA	3515	С		םיב	65	95.441	23.832			D
ATOM	3516	0	VAI	r D	65	95.783	22.961	20.746	1.00 23.24	
ATOM	3517	N	LE	ם נ	66	95.552	25.133	21.271	1.00 25.03	D
MOTA	3518	CA	LE	J D	66	96.102	25.580	19.991	1.00 26.10	D
ATOM	3519	CB		J D	66	96.104	27.111	19.870	1.00 23.98	D
	3520	CG		JD	66	94.826	27.953	19.969	1.00 25.20	D
ATOM			LE		66	95.030	29.233	19.169	1.00 21.70	D
ATOM	3521							19.435	1.00 26.16	D
MOTA	3522		FE		66	93.629	27.211			D
MOTA	3523	C	LE	U D	66	97.533	25.078	19.880	1.00 26.24	
ATOM	3524	0	LE	UD	66	97.971	24.667	18.816	1.00 27.10	D
ATOM	3525	N	LY	S D	67	98.262	25.131	20.989	1.00 27.93	D
MOTA	3526	CA	LY	S D	67	99.642	24.658	21.024	1.00 28.00	D
ATOM	3527	CB		S D		100.215	24.827	22.437	1.00 27.69	D
		CG		s D		101.633	24.316		1.00 28.46	D
MOTA	3528								1.00 30.94	D
MOTA	3529	CD		S D		102.086			1.00 32.95	D
MOTA	3530	CE		SD		103.401				
MOTA	3531	NZ	LY	SD	67	104.517			1.00 35.64	D
ATOM	3532	C	LY	S D	67	99.642	23.182			D
ATOM	3533	0	LY	SD	67	100.414	22.759	19.767	1.00 27.65	D
ATOM	3534			SI		98.761		21.254	1.00 27.05	D
				SI		98.665			1.00 26.31	D
MOTA	3535									D
MOTA	3536			SI		97.600				D
MOTA	3537			SI		97.356				
MOTA	3538		2 HI			97.801				D
MOTA	3539		1 HI	SI	68	96.582	18.466			D
MOTA	3540		1 HI			96.560	17.146	20.423		D
MOTA	3541		2 HI			97.292			1.00 31.58	D
				SI		98.341				D
ATOM	3542					98.958				D
MOTA	3543			S I						D
ATOM	3544			I ME		97.386				D
MOTA	3545			I ME		96.986				
ATOM	3546	CE	AS	en i	69	95.70				D
MOTA	3547		AS	3N 1	D 69	94.44	7 21.504	17.809	1.00 24.20	D

ATOM	3548	CD1	ASN D	69	94.521	20.536	18.562	1.00 26.69	D
ATOM	3549		ASN D	69	93.283	21.994	17.381	1.00 21.03	D
ATOM	3550	C	ASN D	69	98.091	21.855	16.601	1.00 24.52	Ď
		o	ASN D	69	98.329	21.223	15.570	1.00 22.82	D
ATOM	3551 3552	N	LEU D	70	98.763	22.954	16.934	1.00 24.56	D
ATOM			TEC D	70	99.831	23.459	16.078	1.00 26.89	D
ATOM	3553	CA	TEO D	70	100.478	24.707	16.690	1.00 23.85	۵
ATOM	3554	CB			101.619	25.306	15.857	1.00 22.71	D
ATOM	3555	CG	TEO D	70		25.776	14.519	1.00 19.18	D
MOTA	3556		LEU D	70	101.082	26.472	16.592	1.00 23.62	D
MOTA	3557		LEU D	70	102.254		15.882	1.00 28.63	D
ATOM	3558	C	LEU D	70	100.900	22.388		1.00 27.56	Ď
MOTA	3559	0	TEO D	70	101.413	22.210	14.780 16.967	1.00 27.30	D
MOTA	3560	N	ASN D	71	101.224	21.687		1.00 35.25	Ď
MOTA	3561	CA	ASN D	71	102.238	20.637	16.962	1.00 35.25	D
ATOM	3562	СВ	ASN D	71	102.393	20.052	18.370	1.00 38.03	D
MOTA	3563	CG	ASN D	71	103.149	20.978	19.307	1.00 40.05	D
ATOM	3564		ASN D	71	103.197	20.751	20.518		D
MOTA	3565		asn d	71	103.752	22.026	18.748	1.00 38.78	D
MOTA	3566	С	ASN D	71	101.931	19.521	15.975	1.00 36.85	
MOTA	3567	0	asn d	71	102.829	18.997	15.316	1.00 36.91	D D
MOTA	3568	N	SER D	72	100.660	19.157	15.876	1.00 38.08	
MOTA	3569	CA	SER D	72	100.261	18.104	14.961	1.00 39.44	D
ATOM	3570	CB	SER D	72	98.847	17.623	15.306	1.00 40.69	D
MOTA	3571	OG	ser d	72	98.529	16.427	14.611	1.00 44.84	D
MOTA	3572	С	SER D	72	100.320	18.614	13.520	1.00 39.55	D C
MOTA	3573	0	SER D	72	100.798	17.915	12.625	1.00 38.61	D
MOTA	3574	N	TRO D	73	99.846	19.839	13.305	1.00 40.64	D
MOTA	3575	CA	TEO D	73	99.844	20.443	11.974	1.00 42.19	D
ATOM	3576	CB	TEA D	73	99.085	21.768	11.990	1.00 42.17	g
ATOM	3577	CG	LEU D	73	97.608	21.700	11.608	1.00 43.12	D
ATOM	3578		PEA D	73	96.891	20.664	12.443	1.00 44.19	D
MOTA	3579	CD2	PER D	73	96.988	23.072	11.801	1.00 44.59	D
ATOM	3580	C	TEA D	73	101.237	20.678	11.407	1.00 43.27	D
MOTA	3581	0	TEA D	73	101.466	20.479	10.215	1.00 43.00	D
MOTA	3582	N	ILE D	74	102.162	21.116	12.253	1.00 44.60	D
ATOM	3583	CA	ILE D	74	103.529	21.364	11.812	1.00 46.44	D
MOTA	3584	CB	ILE D	74	104.431	21.770	13.000	1.00 46.31	D
MOTA	3585	CG2	ILE D	74	105.893	21.792	12.571	1.00 46.14	D
MOTA	3586	CG1	ILE D	74	103.996	23.140	13.529	1.00 45.97	D
MOTA	3587	CD1	ILE D	74	104.683	23.561	14.812	1.00 43.97	D
MOTA	3588	C	ILE D	74	104.077	20.095	11.166	1.00 48.14	D
ATOM	3589	0	IPE D	74	104.724	20.147	10.119	1.00 48.28	D
MOTA	3590	N	LYS D	75	103.800	18.957	11.795	1.00 49.68	D
ATOM	3591	CA	LYS D	75	104.252	17.669	11.290	1.00 51.82	D
ATOM	3592	CB	LYS D	75	104.060	16.589	12.356	1.00 52.85	D
ATOM	3593	CG	LYS D	75	104.856	16.839	13.621	1.00 54.78	D
ATOM	3594	CD	LYS D	75	104.517	15.831	14.704	1.00 57.28	D
ATOM	3595	CE	LYS D	75	105.222	16.170	16.010	1.00 58.75	D
MOTA	3596	NZ	LYS D	75	104.803	15.266	17.116	1.00 59.97	D
MOTA	3597	C	LYS D	75	103.499	17.276	10.023	1.00 52.37	D
MOTA	3598	0	LYS D	75	104.106	17.086	8.972	1.00 52.78	ם
ATOM	3599	N	ARG D	76	102.177	17.171	10.124	1.00 52.67	ם
MOTA	3600	CA	ARG D	76	101.353	16.783	8.986	1.00 52.67	D
MOTA	3601	CB	ARG D	76	99.911	16.546	9.439	1.00 53.54	D
MOTA	3602	CG	ARG D	76	99.764	15.339	10.346	1.00 55.62	D
MOTA	3603	CD	ARG D	76	98.310	15.011	10.639	1.00 58.29	D
ATOM	3604	NE	ARG D	76	97.628	16.107	11.319	1.00 61.07	D
MOTA	3605	CZ	ARG D	76	96.437	16.000	11.900	1.00 62.21	D
ATOM	3606	NH:	L ARG D	76	95.793	14.840	11.885	1.00 62.71	D
ATOM	3607	NH	2 ARG D	76	95.889	17.055	12.492	1.00 61.94	D
MOTA	3608	C	ARG D	76	101.375	17.761	7.816	1.00 52.35	D
MOTA	3609	0	ARG I	76	100.691	17.550	6.817	1.00 52.65	ם
MOTA	3610	N	SER I	77	102.160	18.824	7.932	1.00 52.02	D
ATOM	3611	CA	SER I	77	102.255	19.807	6.856	1.00 51.87	D
ATOM	3612		SER I		101.945	21.212	7.379	1.00 50.95	D
ATOM	3613		SER I	77	102.975		8.239	1.00 48.11	D
ATOM	3614		SER I		103.667	19.789	6.287	1.00 52.25	a
ATOM	3615		SER I	77	104.028		5.464	1.00 51.67	D
ATOM	3616		ASN I		104.455		6.731	1.00 52.79	D
ATOM	3617				105.841	18.675	6.301	1.00 53.67	D
ATOM	3618				105.912	18.364		1.00 55.53	D
MOTA	3619				107.298			1.00 57.31	D
ATOM	3620		1 ASN 1		107.959			1.00 56.41	D
ATOM	3621		2 ASN 1	78	107.732	18.360	3.184	1.00 58.05	D

ATOM	3622	C	ASN	n	78	106.549	19.985	6.632	1.00 52.90	D
ATOM	3623	0	ASN		78	107.300	20.536	5.826	1.00 53.98	D
	3624	N	SER		79	106.275	20.479	7.835	1.00 51.25	D.
ATOM							21.715	8.341	1.00 49.59	D
MOTA	3625	CA	SER		79	106.856		8.664	1.00 49.69	D
ATOM	3626	CB	SER		79	108.333	21.498	9.753	1.00 52.23	D
ATOM	3627	OG	SER		79	108.472	20.604		1.00 32.23	D
ATOM	3628	С	SER		79	106.711	22.931	7.437		
ATOM	3629	0	SER		79	107.699	23.588	7.111	1.00 47.49	D
MOTA	3630	N	THR		80	105.483	23.235	7.032	1.00 44.68	D
ATOM	3631	CA	THR		80	105.245	24.401	6.189	1.00 43.69	D
ATOM	3632	CB	THR	D	80	103.928	24.274	5.407	1.00 45.12	D
ATOM	3633	OG1	THR	D	80	103.976	23.112	4.570	1.00 47.94	ם
MOTA	3634	CG2	THR	D	80	103.706	25.505	4.541	1.00 44.11	D
ATOM	3635	C	THR	D	80	105.166	25.634	7.094	1.00 42.94	D
ATOM	3636	0	THR	D	80	104.225	25.783	7.874	1.00 41.60	D
ATOM	3637	N	ALA	D	81	106.162	26.510	6.988	1.00 40.39	D
MOTA	3638	CA	ALA	D	81	106.215	27.715	7.804	1.00 37.86	D
ATOM	3639	CB	ALA		81	107.657	28.171	7.958	1.00 39.23	D
ATOM	3640	C	ALA		81	105.372	28.846	7.234	1.00 36.29	D
ATOM	3641	ŏ	ALA		81	104.988	28.829	6.065	1.00 35.21	D
MOTA	3642	N	ALA		82	105.087	29.829	8.079	1.00 34.40	D
	3643	CA	ALA		82	104.294	30.984	7.685	1.00 32.51	D
ATOM		СВ	ALA		82	103.915	31.789	8.920	1.00 32.45	D
MOTA	3644					105.064	31.866	6.707	1.00 32.78	D
ATOM	3645	C	ALA		82				1.00 32.70	D
MOTA	3646	0	ALA		82	106.294	31.913	6.740		ם
ATOM	3647	N	THR		83	104.333	32.561	5.839	1.00 32.79	D
MOTA	3648	CA	THR		83	104.940	33.459	4.867	1.00 34.48	
MOTA	3649	CB	THR		83	104.195	33.429	3.521	1.00 35.64	D
ATOM	3650		THR		83	104.179	32.094	3.006	1.00 38.88	D
ATOM	3651	CG2	THR	D	83	104.880	34.342	2.521	1.00 35.33	D
MOTA	3652	C	THR	D	83	104.886	34.887	5.401	1.00 35.30	D
MOTA	3653	0	THR	D	83	103.827	35.355	5.824	1.00 36.88	D
MOTA	3654	N	ASN	D	84	106.025	35.575	5.379	1.00 35.07	D
MOTA	3655	CA	ASN	D	84	106.095	36.949	5.855	1.00 33.90	D
MOTA	3656	CB	ASN	D	84	107.548	37.413	6.010	1.00 34.23	D
ATOM	3657	CG	ASN		84	108.351	36.545	6.954	1.00 36.16	D
ATOM	3658		ASN		84	107.895	36.195	8.043	1.00 34.99	D
ATOM	3659		ASN		84	109.572	36.205	6.545	1.00 37.40	D
ATOM	3660	C	ASN		84	105.419	37.879	4.865	1.00 34.74	D
ATOM	3661	ō	ASN		84	105.814	37.940	3.699	1.00 35.59	D
ATOM	3662	N	GLU		85	104.401	38.599	5.327	1.00 34.09	D
		CA	GLU		85	103.695	39.561	4.489	1.00 32.99	D
ATOM	3663				85	102.239	39.714	4.939	1.00 35.56	D
ATOM	3664	CB	GLU		85	101.370	38.475	4.746	1.00 40.80	D
MOTA	3665	CG	GLU			101.019	38.215	3.291	1.00 43.32	D
MOTA	3666	CD	GLU		85		39.104	2.658	1.00 46.21	D
MOTA	3667		. GLU		85	100.409	37.119	2.782	1.00 44.58	D
MOTA	3668		GLU		85	101.345			1.00 31.21	D
ATOM	3669	C	GLU		85	104.418	40.886	4.681		D
MOTA	3670	0	GLU		85	105.220	41.024	5.602	1.00 32.36	
MOTA	3671	N	VAL		86	104.140	41.848	3.808	1.00 29.71	D
ATOM	3672	CA	VAL		86	104.749	43.170	3.882	1.00 27.94	D
MOTA	3673	CB	VAL	D	86	105.079	43.712	2.467	1.00 26.90	D
ATOM	3674	CG1	LVAL	D	86	105.569	45.166	2.543	1.00 23.11	D
MOTA	3675	CG2	VAL	D	86	106.134	42.829	1.821	1.00 24.31	D
MOTA	3676	C	VAL	D	86	103.767	44.114	4.574	1.00 29.81	D
MOTA	3677	0	VAL	D	86	102.658	44.343	4.088	1.00 30.28	D
ATOM	3678	N	PRO		87	104.162	44.666	5.729	1.00 29.08	D
ATOM	3679	CD	PRO		87	105.356	44.310	6.509	1.00 29.37	D
MOTA	3680	CA	PRO		87	103.306	45.583	6.485	1.00 30.85	D
ATOM	3681	CB	PRO		87	104.083	45.791	7.786	1.00 30.80	D
MOTA	3682	CG	PRO		87	104.878	44.551	7.920	1.00 30.83	D
ATOM	3683	C	PRO		87	103.049	46.907	5.772	1.00 31.43	D
			PRO			103.863	47.357	4.968	1.00 31.78	D
MOTA	3684	0			87		47.517	6.081	1.00 31.85	D
MOTA	3685	N	GLU		88	101.907	48.808	5.521	1.00 32.77	D
MOTA	3686	CA	GLU		88	101.516			1.00 32.77	D
MOTA	3687	CB	GLU		88	100.195	48.687	4.744		ם
MOTA	3688	CG	GLU		88	99.814	49.960	3.987	1.00 43.00	
ATOM	3689	æ			88	98.512	49.839	3.205	1.00 46.30	D
ATOM	3690		1 GLU		88	97.439	49.745	3.837	1.00 47.40	D
MOTA	3691	OE:	2 GLU	J D	88	98.564	49.840	1.954	1.00 48.25	D
MOTA	3692	C	GL/	ם נ	88	101.338	49.748	6.721	1.00 31.26	D
MOTA	3693	0	GL	ם נ	88	100.556	49.457	7.630	1.00 31.21	D
MOTA	3694		VAI	םי	89	102.060	50.864	6.728	1.00 28.43	D
MOTA	3695		VAI	ם	89	101.988	51.806	7.842	1.00 26.87	ם

				_			ra aa4	0 454	1.00 26.58	ם
ATOM	3696	СВ	VAL I		89	103.385	52.024	8.454		
MOTA	3697	CG1	VAL 1		89	103.277	52.886	9.699	1.00 26.80	ם
ATOM	3698	CG2	VAL 1	כ	89	104.021	50.679	8.787	1.00 24.58	מ
ATOM	3699	C	VAL I	0	89	101.389	53.174	7.505	1.00 27.02	D
ATOM	3700	0	VAL I	D	89	101.698	53.772	6.473	1.00 26.22	D
ATOM	3701	N	THR		90	100.530	53.662	8.394	1.00 26.33	D
						99.881	54.955	8.219	1.00 26.05	D
ATOM	3702	CA	THR I		90					
MOTA	3703	CB	THR I		90	98.414	54.802	7.769	1.00 27.24	D
ATOM	3704	OG1	THR I	D	90	98.359	54.063	6.543	1.00 31.41	D
ATOM	3705	CG2	THR I	D	90	97.786	56.163	7.545	1.00 28.57	· D
MOTA	3706	C	THR I	D	90	99.883	55.698	9.546	1.00 24.83	D
ATOM	3707	ō	THR		90	99.542	55.120	10.581	1.00 25.45	D
						100.266	56.972	9.512	1.00 22.04	D
ATOM	3708	N	VAL I		91					D
ATOM	3709	CA	VAL 1		91	100.300	57.791	10.716	1.00 21.50	
ATOM	3710	CB	VAL I	D	91	101.749	58.280	11.031	1.00 23.04	D
ATOM	3711	CG1	VAL 1	D	91	101.737	59.245	12.225	1.00 22.74	D
ATOM	3712	CG2	VAL:	D	91	102.650	57.082	11.340	1.00 20.38	D
MOTA	3713	С	VAL :	D	91	99.369	58.993	10.553	1.00 21.65	D
ATOM	3714	ō	VAL		91	99.357	59.653	9.509	1.00 21.70	D
			PHE		92	98.573	59.252	11.586	1.00 21.34	D
ATOM	3715	N							1.00 21.48	D
ATOM	3716	CA	PHE		92	97.633	60.363	11.580		
ATOM	3717	CB	PHE	D	92	96.370	59.985	10.788	1.00 21.60	D
MOTA	3718	CG	PHE	D	92	95.652	58.771	11.314	1.00 22.22	D
MOTA	3719	CD1	PHE	D	92	94.601	58.902	12.215	1.00 24.10	D
MOTA	3720	CD2	PHE	D	92	96.038	57.495	10.925	1.00 24.53	D
ATOM	3721		PHE		92	93.940	57.774	12,724	1.00 22.72	D
						95.386	56.355	11.428	1.00 23.87	D
ATOM	3722		PHE		92					D
MOTA	3723	cz	PHE		92	94.335	56.501	12.329	1.00 21.18	
MOTA	3724	C	PHE	D	92	97.303	60.700	13.030	1.00 22.72	D
MOTA	3725	0	PHE	D	92	97.607	59.921	13.933	1.00 22.31	D
MOTA	3726	N	SER	D	93	96.696	61.859	13.261	1.00 22.45	D
ATOM	3727	CA	SER		93	96.366	62.262	14.623	1.00 21.69	D
ATOM	3728	СВ	SER		93	96.599	63.764	14.799	1.00 20.96	D
					93	95.696	64.508	14.010	1.00 25.08	D
MOTA	3729	OG	SER						1.00 21.02	D
MOTA	3730	С	SER		93	94.931	61.913	14.990		
ATOM	3731	0	SER	Ð	93	94.078	61.755	14.127	1.00 20.62	D
ATOM	3732	N	LYS	D	94	94.676	61.791	16.283	1.00 20.66	D
ATOM	3733	CA	LYS	D	94	93.350	61.453	16.768	1.00 24.11	D
ATOM	3734	CB	LYS	D	94	93.444	60.985	18.223	1.00 24.91	D
ATOM	3735	CG	LYS		94	92.121	60.605	18.865	1.00 29.49	D
			LYS		94	92.353	60.101	20.293	1.00 32.97	D
ATOM	3736	CD .							1.00 33.37	D
MOTA	3737	CE	LYS		94	91.050	59.909	21.052		
MOTA	3738	NZ	LYS		94	90.175	58.897	20.399	1.00 34.08	D
ATOM	3739	С	LYS	D	94	92.406	62.646	16.654	1.00 24.40	D
ATOM	3740	0	LYS	D	94	91.224	62.495	16.356	1.00 24.55	D
ATOM	3741	N	SER	D	95	92.935	63.834	16.894	1.00 25.54	D
ATOM	3742	CA	SER		95	92.133	65.040	16.815	1.00 29.22	D
						91.932	65.643	18.208	1.00 30.47	D
ATOM	3743	CB	SER		95				1.00 36.11	D
ATOM	3744	OG	SER		95	91.236	64.746	19.060		
ATOM	3745	C	SER	D	95	92.843	66.046	15.932	1.00 29.71	D
ATOM	3746	0	SER	D	95	93.993	65.834	15.531	1.00 29.68	D
ATOM	3747	N	PRO	D	96	92.159	67.146	15.588	1.00 29.93	D
ATOM	3748	8	PRO	D	96	90.760	67.532	15.843	1.00 31.14	D
MOTA	3749	CA	PRO		96	92.836	68.129	14.747	1.00 29.29	D
	3750	CB	PRO		96	91.714	69.097	14.369	1.00 31.65	D
MOTA							69.010	15.545	1.00 30.66	D
MOTA	3751	CG	PRO		96	90.777				
MOTA	3752	C	PRO		96	93.939	68.765	15.587	1.00 27.35	D
ATOM	3753	0	PRO	D	96	93.818	68.904	16.806	1.00 24.86	D
ATOM	3754	N	VAL	D	97	95.025	69.127	14.929	1.00 26.81	D
MOTA	3755	CA	VAL		97	96.158	69.706	15.615	1.00 29.25	D
ATOM	3756	CB	VAL		97	97.438	69.501	14.783	1.00 31.49	D
						98.652	69.998	15.556	1.00 33.50	D
MOTA	3757		L VAL		97				1.00 34.03	D
MOTA	3758		2 VAL		97	97.583	68.029	14.415		
MOTA	3759	C	VAL		97	96.007	71.196	15.910	1.00 28.80	D
ATOM	3760	0	VAL	D	97	95.749	71.998	15.012	1.00 28.78	D
MOTA	3761	N	THR		98	96.144	71.559	17.178	1.00 27.47	D
ATOM	3762	CA	THR		98	96.091	72.960	17.572	1.00 26.55	D
ATOM	3763	СВ	THR		98	94.723		18.209	1.00 26.16	D
ATOM	3764		1 THR		98	94.684	_	19.575	1.00 31.83	D
								17.469	1.00 23.66	D
MOTA	3765		2 THR		98	93.567			1.00 25.73	D
MOTA	3766	C	THR		98	97.220	_	18.581		
MOTA	3767	0	THR	D	98	97.260		19.591	1.00 27.12	D
MOTA	3768	N	LEU	D	99	98.159		18.285	1.00 26.12	D
MOTA	3769	CA	LEU	D	99	99.307	74.236	19.156	1.00 27.47	D

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ATOM	3770	CB	LEU D	99	100.089	75.459	18.675	1.00 31.04	D
ATOM	3771	CG	TEA D	99	100.758	75.309	17.310	1.00 33.09	D
ATOM	3772	CD1	LEU D	99	101.458	76.607	16.940	1.00 36.20	D
ATOM	3773		LEU D	99	101.754	74.165	17.361	1.00 35.56	D
			LEU D	99	98.935	74.416	20.621	1.00 26.08	D
ATOM	3774	C						1.00 25.97	D
ATOM	3775	0	TEO D	99	98.077	75.222	20.946		
ATOM	3776	N	GLY D	100	99.585	73.654	21.500	1.00 26.97	D
MOTA	3777	CA	GLY D	100	99.310	73.749	22.924	1.00 26.03	D
ATOM	3778	C	GLY D	100	98.233	72.798	23.422	1.00 26.02	D
		ō	GLY D		98.020	72.662	24.629	1.00 25.51	D
MOTA	3779		-				22.491	1.00 25.73	D
ATOM	3780	N	GLN D		97.553	72.143			
MOTA	3781	CA	GLN D	101	96.490	71.199	22.820	1.00 28.13	D
ATOM	3782	CB	GLN D	101	95.372	71.297	21.776	1.00 32.24	D
ATOM	3783	CG	GLN D	101	94.617	69.981	21.560	1.00 38.65	ם
ATOM	3784	CD	GLN D		94.680	69.459	20.115	1.00 41.08	D
					95.760	69.348	19.511	1.00 38.18	D
MOTA	3785	OE1							D
ATOM	3786	NE2	GLN D		93.515	69.119	19.566	1.00 40.87	
ATOM	3787	С	GFM D	101	96.994	69.756	22.861	1.00 25.22	D
MOTA	3788	0	GLN D	101	97.477	69.245	21.857	1.00 24.55	D
ATOM	3789	N	PRO D	102	96.885	69.078	24.019	1.00 24.18	D
		ĊD.	PRO D		96.436	69.544	25.343	1.00 22.22	D
ATOM	3790					67.683	24.080	1.00 22.76	D
MOTA	3791	CA	PRO D		97.359				D
ATOM	3792	CB	PRO D		96.983	67.253	25.494	1.00 22.02	
ATOM	3793	CG	PRO D	102	97.088	68.542	26.274	1.00 22.44	ם
ATOM	3794	C	PRO D	102	96.649	66.845	23.015	1.00 21.72	ם
	3795	ō	PRO D	102	95.429	66.922	22.876	1.00 22.65	D
MOTA					97.409	66.055	22.264	1.00 19.84	D
MOTA	3796	N	ASN D						D
MOTA	3797	CA	asn d		96.833	65.225	21.209	1.00 17.89	
ATOM	3798	CB	ASN D	103	97.112	65.856	19.838	1.00 16.30	D
MOTA	3799	CG	ASN D	103	96.005	65.587	18.824	1.00 16.50	D
ATOM	3800		ASN D		95.552	64.446	18.636	1.00 16.80	D
			ASN D		95.569	66.643	18.160	1.00 14.61	D
MOTA	3801					63.805	21.248	1.00 17.24	D
ATOM	3802	С	ASN D		97.410				D
MOTA	3803	0	ASN D		98.199	63.473	22.129	1.00 15.74	
MOTA	3804	N	ILE D	104	97.010	62.977	20.284	1.00 17.39	D
ATOM	3805	CA	ILE D	104	97.465	61.595	20.198	1.00 15.30	D
ATOM	3806	CB	IFE D	104	96.402	60.627	20.755	1.00 17.89	D
		CG2			96.818	59.175	20.498	1.00 13.27	D
ATOM	3807						22.253	1.00 18.46	D
ATOM	3808		ILE D		96.202	60.886			
ATOM	3809	CD1	ILE D	104	95.179	59.965	22.895	1.00 17.98	D
ATOM	3810	C	ILE D	104	97.760	61.185	18.763	1.00 17.15	Ď
ATOM	3811	0	ILE D	104	96.887	61.283	17.902	1.00 18.07	D
ATOM	3812	N	LEU D		98.987	60.727	18.509	1.00 16.66	D
			LEU D		99.370	60.272	17.177	1.00 16.59	D
MOTA	3813	CA					16.895	1.00 17.56	D
MOTA	3814	CB	TER D		100.864	60.482			Ď
MOTA	3815	CG	TEA D	105	101.375	61.926	16.842	1.00 21.66	
ATOM	3816	CD1	LEU D	105	102.811	61.943	16.302	1.00 21.26	D
ATOM	3817	CD2	LEU D	105	100.460	62.771	15.951	1.00 21.56	D
ATOM	3818	C	LEU D		99.061	58.804	17.128	1.00 17.13	D
			TEA D		99.368	58.056	18.056	1.00 18.35	D
MOTA	3819	0			98.432	58.399	16.039	1.00 17.88	D
MOTA	3820	N	ILE D						D
MOTA	3821	CA	ILE D	106	98.045	57.016	15.839	1.00 17.14	
MOTA	3822	CB	ILE D	106	96.525	56.939	15.492	1.00 16.99	D
ATOM	3823	CG2	ILE D	106	96.093	55.496	15.318	1.00 15.63	D
ATOM	3824		LILED		95.711	57.619	16.604	1.00 19.04	D
			LILED		94.238	57.877	16.260	1.00 16.48	D
MOTA	3825				98.876	56.431	14.700	1.00 17.19	D
MOTA	3826	C	ILE D					1.00 16.06	D
MOTA	3827	0	ILE D	106	98.941	57.004	13.618		
ATOM	3828	N	CYS D	107	99.540	55.312	14.966	1.00 18.84	D
ATOM	3829	CA	CYS D	107	100.339	54.637	13.954	1.00 19.74	D
ATOM	3830	C	CYS D		99.634	53.323	13.670	1.00 20.17	D
			CYS I		99.632	52.421	14.507	1.00 20.08	ם
MOTA	3831	0				54.349		1.00 22.00	D
MOTA	3832	CB	CYS D		101.755		14.453	1.00 28.61	D
ATOM	3833	SG	CYS I		102.800	53.514	13.211		
MOTA	3834	N	LEU I	108	99.027	53.221	12.493	1.00 19.48	מ
MOTA	3835	CA	LEU I	108	98.313	52.015	12.113	1.00 19.67	D
ATOM	3836	CB			97.024	52.391	11.369	1.00 19.98	ם
					95.977	51.358	10.925	1.00 20.40	D
MOTA	3837	CG				51.366	9.412	1.00 20.15	D
MOTA	3838		1 LEU I		95.883				D
MOTA	3839	CD	2 LEU I	108	96.301	49.971	11.454	1.00 19.44	
MOTA	3840	С	LEU I	108	99.207	51.145	11.237	1.00 19.84	D
ATOM	3841		LEU I	108	99.657	51.563	10.170	1.00 20.11	D
ATOM	3842	N	VAL I		99.473	49.940	11.721	1.00 19.32	D
MOTA	3843	CA			100.289	48.972	11.016		D
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ATOM	3844	CB	VAL D 109	101.368	48.402	11.958	1.00 19.40	D
ATOM	3845		VAL D 109		47.474	11.202	1.00 18.01	ם
ATOM	3846		VAL D 109		49.560	12.590	1.00 17.30	D
ATOM	3847	C	VAL D 109		47.876	10.568	1.00 21.45	D
ATOM	3848	Ō	VAL D 109		47.079	11.382	1.00 22.65	D
ATOM	3849	N	ASP D 110		47.861	9.274	1.00 22.00	D
ATOM	3850	CA	ASP D 110		46.901	8.689	1.00 23.80	D
ATOM	3851	СВ	ASP D 110		47.648	7.728	1.00 24.68	D
ATOM	3852	CG	ASP D 110		47.002	7.603	1.00 26.64	D
ATOM	3853		ASP D 110		45.915	8.177	1.00 28.80	Œ
ATOM	3854		ASP D 110		47.591	6.926	1.00 27.99	Œ
ATOM	3855	c	ASP D 110		45.756	7.944	1.00 23.77	D
ATOM	3856	ō	ASP D 110		45.831	7.684	1.00 22.82	D
ATOM	3857	N	ASN D 11:		44.711	7.604	1.00 23.55	D
ATOM	3858	CA	ASN D 11:		43.530	6.889	1.00 23.79	D
ATOM	3859	CB	ASN D 11:		43.867	5.425	1.00 25.36	D
ATOM	3860	CG	ASN D 11:		42.610	4.562	1.00 29.95	D
ATOM	3861		ASN D 11:		42.547	3.724	1.00 29.58	D
ATOM	3862	ND2			41.611	4.761	1.00 30.51	D
ATOM	3863	C	ASN D 11:	99.786	42.941	7.556	1.00 22.70	D
ATOM	3864	0	ASN D 11:	100.834	42.784	6.929	1.00 22.97	D
MOTA	3865	N	ILE D 11:	99.656	42.612	8.835	1.00 22.14	D
ATOM	3866	CA	ILE D 11:	100.754	42.03B	9.598	1.00 20.20	D
ATOM	3867	CB	ILE D 11:	100.746	42.536	11.055	1.00 18.82	ם
ATOM	3868	CG2	ILE D 11:	101.926	41.950	11.808	1.00 15.77	D
ATOM	3869	CG1	ILE D 11	100.770	44.058	11.103	1.00 19.09	D
ATOM	3870	CD1	ILE D 11	100.630	44.602	12.514	1.00 21.18	D
ATOM	3871	C	ILE D 11	100.666	40.512	9.659	1.00 21.41	D
MOTA	3872	0	ILE D 11	99.626	39.960	10.002	1.00 22.04	D
MOTA	3873	N	PHE D 11	3 101.765	39.838	9.338	1.00 21.35	D
ATOM	3874	CA	PHE D 11		38.386	9.409	1.00 19.93	D
ATOM	3875	CB	PHE D 11		37.726	8.462	1.00 21.28	D
MOTA	3876	CG	PHE D 11		36.306	8.825	1.00 20.91	D
MOTA	3877		PHE D 11		36.012	9.838	1.00 19.85	D
MOTA	3878		PHE D 11		35.261	8.230	1.00 22.61	D
MOTA	3879		PHE D 11		34.698	10.264	1.00 20.63	D
MOTA	3880	CE2			33.942	8.646	1.00 21.21	D
MOTA	3881	CZ	PHE D 11		33.660	9.669	1.00 20.87	D
MOTA	3882	C	PHE D 11		37.871	9.071	1.00 19.98 1.00 20.80	D D
ATOM	3883	0	PHE D 11		38.238	8.044 9.925	1.00 20.00	D
MOTA	3884	N	PRO D 11		37.005 36.414	9.732	1.00 21.20	D
MOTA	3885	CD.	PRO D 11 PRO D 11		36.518	11.166	1.00 21.41	D
MOTA	3886 3887	CA CB	PRO D 11		35.424	11.625	1.00 21.03	D
ATOM ATOM	3888	CG	PRO D 11		35.912	11.115	1.00 22.98	D
ATOM	3889	C	PRO D 11		37.648	12.185	1.00 21.84	D
ATOM	3890	ŏ	PRO D 11		38.711	12.034	1.00 20.41	D
ATOM	3891	N	PRO D 11			13.222	1.00 22.52	D
ATOM	3892	CD	PRO D 11		36.256	13.445	1.00 22.08	D
ATOM	3893	CA	PRO D 11		38.448	14.266	1.00 21.19	D
ATOM	3894	CB	PRO D 11			15.025	1.00 20.92	D
ATOM	3895	CG	PRO D 11			14.902	1.00 19.88	D
ATOM	3896	C	PRO D 11		38.683	15.171	1.00 21.62	D
ATOM	3897	ō	PRO D 11			16.356	1.00 22.92	D
MOTA	3898	N	VAL D 11	6 104.179	39.263	14.588	1.00 21.58	D
ATOM	3899	CA	VAL D 11	6 105.405	39.598	15.300	1.00 22.53	Q
ATOM	3900	СВ	VAL D 11	6 106.520	38.554	15.067	1.00 24.90	Ď
MOTA	3901	CG1	VAL D 11	6 107.817	39.035	15.713	1.00 24.06	D
MOTA	3902	CG2	VAL D 11	6 106.104	37.195	15.641	1.00 24.88	D
ATOM	3903	С	VAL D 11	6 105.855	40.929	14.708	1.00 21.86	. р
ATOM	3904	0	VAL D 11			13.509	1.00 20.87	D
MOTA	3905	N	VAL D 11	.7 105.935		15.534	1.00 20.65	D
MOTA	3906	CA	VAL D 11				1.00 21.60	D
MOTA	3907	CB	VAL D 1				1.00 18.11	D
ATOM	3908		L VAL D 13				1.00 16.63	D
ATOM	3909		VAL D 1				1.00 17.02	D
MOTA	3910	C	VAL D 1				1.00 23.84	D
ATOM	3911	0	VAL D 1				1.00 24.78	D
MOTA	3912	N	ASN D 1				1.00 27.93	D.
MOTA	3913	CA	ASN D 1				1.00 30.45	D D
MOTA	3914	CB	ASN D 1				1.00 33.93 1.00 39.88	D
ATOM	3915	CG	ASN D 1				1.00 39.88	ם
ATOM	3916		1 ASN D 1				1.00 42.45	D
MOTA	3917	ND	2 ASN D 1:			20.0.0		_

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ATOM	3918	C	ASN D 118	107.960		16.181	1.00 27.72	D
ATOM	3919	0	ASN D 118	108.398	47.952	15.140	1.00 26.88	D
MOTA	3920	N	ILE D 119	107.126	48.113	16.988	1.00 27.59	D
ATOM	3921	CA	ILE D 119	106.680	49.476	16.700	1.00 27.12	D
ATOM	3922	CB	ILE D 119	105.133		16.719	1.00 27.17	D
			ILE D 119	104.698		16.346	1.00 26.16	D
MOTA	3923			104.528		15.741	1.00 24.63	D
ATOM	3924		ILE D 119		48.572			D
ATOM	3925	CD1	ILE D 119	103.026	48.423	15.877	1.00 24.19	
MOTA	3926	C	ILE D 119	107.243	50.436	17.746	1.00 27.72	ם
MOTA	3927	0	ILE D 119	107.050	50.248	18.946	1.00 26.86	D
MOTA	3928	N	THR D 120	107.951	51.460	17.291	1.00 27.54	D
ATOM	3929	CA	THR D 120	108.524	52.423	18.214	1.00 29.37	D
ATOM	3930	CB	THR D 120	110.022	52.131	18.477	1.00 32.22	D
			THR D 120	110.722	52.034	17.229	1.00 35.14	D
MOTA	3931				50.817	19.247	1.00 35.67	D
ATOM	3932		THR D 120	110.176			1.00 27.95	D
ATOM	3933	C	THR D 120	108.369	53.826	17.668		
MOTA	3934	0	THR D 120	108.398	54.035	16.459	1.00 29.89	D
ATOM	3935	N	TRP D 121	108.187	54.789	18.560	1.00 26.28	D
ATOM	3936	CA	TRP D 121	108.031	56.171	18.135	1.00 26.93	D
ATOM	3937	CB	TRP D 121	106.935	56.866	18.940	1.00 24.20	D
ATOM	3938	CG	TRP D 121	105.568	56.343	18.687	1.00 22.03	D
ATOM	3939		TRP D 121	104.643	56.826	17.707	1.00 20.30	D
		CE2		103.454	56.085	17.856	1.00 20.70	D
MOTA	3940		TRP D 121	104.705	57.817	16.717	1.00 17.15	D
MOTA	3941						1.00 21.06	D
MOTA	3942		TRP D 121	104.929	55.351	19.365		D
MOTA	3943		TRP D 121	103.655	55.190	18.875	1.00 22.39	
MOTA	3944	CZ2	TRP D 121	102.332	56.305	17.057	1.00 17.25	D
ATOM	3945	CZ3	TRP D 121	103.593	58.036	15.924	1.00 17.92	D
ATOM	3946	CH2	TRP D 121	102.419	57.282	16.099	1.00 19.11	D
ATOM	3947	C	TRP D 121	109.319	56.957	18.284	1.00 26.88	D
	3948	ō	TRP D 121	110.059	56.789	19.251	1.00 27.48	D
ATOM			LEU D 122	109.572	57.830	17.321	1.00 29.82	D
MOTA	3949	N	LEU D 122	110.764	58.658	17.343	1.00 31.91	D
MOTA	3950	CA					1.00 34.65	D
MOTA	3951	CB	LEU D 122	111.664	58.331	16.144		
MOTA	3952	CG	LEU D 122	112.391	56.977	16.112	1.00 37.28	D
ATOM	3953	CD1	LEU D 122	113.247	56.828	17.360	1.00 37.11	מ
ATOM	3954	CD2	LEU D 122	111.394	55.840	16.025	1.00 39.41	D
ATOM	3955	С	LEU D 122	110.416	60.142	17.324	1.00 31.97	D
ATOM	3956	0	LEU D 122	109.619	60.593	16.503	1.00 31.46	D
ATOM	3957	N	SER D 123	111.010	60.889	18.250	1.00 31.03	Œ
		CA	SER D 123	110.813	62.331	18.326	1.00 33.04	D
MOTA	3958		SER D 123	110.312	62.745	19.712	1.00 32.42	D
MOTA	3959	CB			64.154	19.793	1.00 32.43	D
MOTA	3960	OG	SER D 123	110.169		18.062	1.00 33.10	D
MOTA	3961	С	SER D 123	112.184	62.948			D
ATOM	3962	0	SER D 123	113.108	62.784	18.860	1.00 33.57	
MOTA	3963	N	ASN D 124	112.309	63.646	16.941	1.00 33.51	D
ATOM	3964	CA	ASN D 124	113.575	64.258	16.553	1.00 36.20	D
MOTA	3965	CB	ASN D 124	113.963	65.392	17.510	1.00 34.61	D
ATOM	3966	CG	ASN D 124	112.946	66.512	17.531	1.00 34.17	D
ATOM	3967		L ASN D 124	112.262	66.764	16.539	1.00 34.73	D
			2 ASN D 124	112.850	67.202	18.660	1.00 35.34	D
ATOM	3968		ASN D 124	114.664	63.191	16.561	1.00 37.34	D
ATOM	3969	C		115.747	63.401	17.104	1.00 37.93	D
ATOM	3970	0	ASN D 124				1.00 38.73	ם
MOTA	3971	N	GLY D 125	114.358	62.039	15.970	1.00 39.56	D
ATOM	3972	CA	GLY D 125	115.317	60.951	15.910		
MOTA	3973	С	GLY D 125	115.457	60.131	17.183	1.00 40.55	D
MOTA	3974	0	GLY D 125	116.051	59.054	17.157	1.00 42.52	D
ATOM	3975	N	HIS D 126	114.911	60.622	18.291	1.00 40.35	D
ATOM	3976	CA	HIS D 126	115.009	59.918	19.569	1.00 41.15	D
MOTA	3977	СВ	HIS D 126	115.234	60.923	20.702	1.00 43.51	. D
				116.525	61.678	20.599	1.00 47.67	D
ATOM	3978	CG		116.775	62.997	20.422	1.00 47.36	D
MOTA	3979		2 HIS D 126			20.694	1.00 49.39	D
MOTA	3980		1 HIS D 126	117.757	61.064			
MOTA	3981		1 HIS D 126	118.709	61.973	20.581	1.00 48.59	D
MOTA	3982	NE	2 HIS D 126	118.140	63.154	20.415	1.00 48.17	D
MOTA	3983		HIS D 126	113.794	59.053	19.907	1.00 40.38	D
ATOM	3984		HIS D 126	112.648	59.458	19.706		D
ATOM	3985		SER D 127	114.056	57.863	20.438	1.00 39.11	D
MOTA	3986			112.995	56.939	20.821	1.00 39.54	D
				113.592	55.592	21.232		D
MOTA	3987			114.299		20.159		D
MOTA	3988			112.167		21.979		D
ATOM	3989		SER D 127			22.930		D
MOTA	3990		SER D 127	112.707				D
MOTA	3991	. N	VAL D 128	110.854	57.326	21.894	T.00 30.40	~

ATOM	3992	CA	VAL D 128	109.967	57.800	22.942	1.00 35.00	D
ATOM	3993	CB	VAL D 128	108.699	58.444	22.358	1.00 33.68	D
ATOM	3994	CG1	VAL D 128	107.834	59.001	23.479	1.00 32.31	D
MOTA	3995	CG2	VAL D 128	109.081	59.543	21.383	1.00 32.69	D
MOTA	3996	C	VAL D 128	109.574	56.608	23.790	1.00 34.62 1.00 35.98	D D
MOTA	3997	0	VAL D 128	109.150	55.584 56.743	23.268 25.100	1.00 35.57	D
ATOM	3998	N	THR D 129 THR D 129	109.715 109.393	55.653	26.007	1.00 38.21	D
MOTA	3999 4000	CA CB	THR D 129	110.562	55.410	26.992	1.00 40.63	D
ATOM ATOM	4001		THR D 129	110.184	54.413	27.949	1.00 44.78	D
ATOM	4002		THR D 129	110.929	56.700	27.715	1.00 42.66	Ð
ATOM	4003	C	THR D 129	108.103	55.862	26.799	1.00 36.54	D
ATOM	4004	0	THR D 129	107.359	54.911	27.042	1.00 38.87	D
ATOM	4005	N	GLU D 130	107.833	57.101	27.195	1.00 33.00	D .
MOTA	4006	CA	GLU D 130	106.631	57.401	27.963	1.00 31.03	D D
MOTA	4007	CB	GLU D 130	106.935	58.453	29.039 29.987	1.00 33.90 1.00 38.08	D
MOTA	4008	CG	GLU D 130	108.067 107.809	58.089 56.788	30.731	1.00 43.43	D
MOTA	4009	CD	GLU D 130	106.744	56.672	31.375	1.00 45.61	۵
MOTA MOTA	4010 4011	OB2		108.671	55.879	30.675	1.00 45.67	D
ATOM	4012	C	GLU D 130	105.521	57.922	27.058	1.00 27.87	D
ATOM	4013	ō	GLU D 130	105.795	58.527	26.029	1.00 24.56	D
ATOM	4014	N	GLY D 131	104.272	57.692	27.457	1.00 26.29	D
ATOM	4015	CA	GLY D 131	103.140	58.166	26.679	1.00 25.19	D
MOTA	4016	C	GLY D 131	102.826	57.304	25.474	1.00 24.46	D
MOTA	4017	0	GLY D 131	102.130	57.725	24.559	1.00 23.65	D
MOTA	4018	N	VAL D 132	103.349	56.089	25.476	1.00 22.83 1.00 23.04	D D
MOTA	4019	CA	VAL D 132	103.117	55.169 54.674	24.379 23.784	1.00 22.91	D
MOTA	4020	CB	VAL D 132	104.448 104.182	53.538	22.821	1.00 24.12	D
ATOM	4021		VAL D 132 VAL D 132	105.164	55.816	23.076	1.00 22.85	D
ATOM ATOM	4022 4023	C	VAL D 132	102.326	53.943	24.829	1.00 21.91	D
MOTA	4024	ŏ	VAL D 132	102.535	53.416	25.917	1.00 21.27	D
ATOM	4025	N	SER D 133	101.412	53.499	23.979	1.00 22.08	D
ATOM	4026	CA	SER D 133	100.622	52.307	24.251	1.00 21.07	D
ATOM	4027	CB	SER D 133	99.405	52.637	25.119	1.00 21.95	D
ATOM	4028	OG	SER D 133	98.567	53.595	24.498	1.00 27.01	D
MOTA	4029	С	SER D 133	100.178	51.738	22.908	1.00 21.27	ם ם
MOTA	4030	0	SER D 133	100.344	52.369	21.864 22.926	1.00 19.82 1.00 20.29	D
MOTA	4031	N	GLU D 134	99.627 99.182	50.538 49.938	21.689	1.00 24.12	D
ATOM	4032	CA CB	GLU D 134 GLU D 134	100.370	49.323	20.932	1.00 26.01	D
ATOM ATOM	4033 4034	CG	GLU D 134	100.932	48.045	21.532	1.00 30.80	Ø
ATOM	4035	CD	GLU D 134	102.080	47.480	20.704	1.00 35.43	D
MOTA	4036		L GLU D 134	102.273	46.243	20.702	1.00 36.93	D
ATOM	4037	OE2	2 GLU D 134	102.793	48.278	20.057	1.00 37.66	D
MOTA	4038	C	GLU D 134	98.127	48.882	21.955	1.00 22.81	D
MOTA	4039	0	GLU D 134	97.968	48.416	23.081	1.00 22.94	D D
MOTA	4040	N	THR D 135	97.400	48.522	20.908	1.00 21.95 1.00 20.78	ם
MOTA	4041	CA	THR D 135	96.361	47.519 47.625	21.009 19.843	1.00 20.70	D
ATOM	4042	CB	THR D 135 1 THR D 135	95.368 96.032	47.262	18.623	1.00 22.24	D
MOTA	4043	OG:	2 THR D 135	94.833	49.046	19.721	1.00 18.01	D
MOTA MOTA	4044 4045	CG.	THR D 135	97.037	46.168	20.890	1.00 20.80	D
MOTA	4045	ō	THR D 135	98.259	46.084	20.742	1.00 21.08	D
MOTA	4047	N	SER D 136	96.234	45.116	20.972	1.00 19.11	Ø
ATOM	4048	CA		96.728	43.764	20.790		D
ATOM	4049	CB	SER D 136	95.769	42.755			D
ATOM	4050	OG	SER D 136	95.656				D
MOTA	4051	C	SER D 136	96.665				D D
MOTA	4052		SER D 136	96.325				D
MOTA	4053		PHE D 137	97.002				D
MOTA	4054			96.896 97.652				D
MOTA	4055			99.138	_			D
MOTA MOTA	4056 4057		1 PHE D 137	99.792			1.00 20.23	D
ATOM	4058	CD.	2 PHE D 137	99.894			1.00 17.79	D
ATOM	4059		1 PHE D 137	101.187				D
MOTA	4060		2 PHE D 137	101.291			1.00 19.39	D
ATOM	4061		PHE D 137	101.935				D
MOTA	4062		PHE D 137	95.402				D D
MOTA	4063		PHE D 137	94.823				D
MOTA	4064		LEU D 138	94.786 93.367				D
ATOM	4065	C C	FER D 138	33.36/	46.131			

ATOM	4066	СВ	LEU D 138	92.722	44.175	15.678	1.00 21.40	D
ATOM	4067	CG	LEU D 138	92.452	45.087	16.881	1.00 22.42	D
MOTA	4068	CD1	LEU D 138	91.889	44.277	.18.032	1.00 23.38	D
ATOM	4069	CD2	LEU D 138	93.732	45.764	17.301	1.00 28.68	D
ATOM	4070	C	LEU D 138	93.230	41.982	14.593	1.00 20.56	D
ATOM	4071	0	LEU D 138	93.919	42.244	13.615	1.00 22.27	D
MOTA	4072	N	SER D 139	92.326	41.013	14.586	1.00 20.44 1.00 19.23	ם ם
MOTA	4073	CA	SER D 139	92.143	40.142	13.427 13.788	1.00 19.23	D
ATOM	4074	CB cc	SER D 139 SER D 139	91.222 89.888	38.986 39.443	13.765	1.00 21.32	Ď
ATOM	4075	OG C	SER D 139	91.594	40.802	12.168	1.00 19.43	Ď,
MOTA MOTA	4076 4077	0	SER D 139	91.028	41.893	12.210	1.00 19.49	D .
ATOM	4078	N	LYS D 140	91.755	40.102	11.050	1.00 18.62	D
ATOM	4079	CA	LYS D 140	91.276	40.553	9.749	1.00 19.20	D
ATOM	4080	CB	LYS D 140	92.437	41.058	8.895	1.00 18.92	D
ATOM	4081	CG	LYS D 140	93.286	42.126	9.554	1.00 19.38	D
ATOM	4082	CD	LYS D 140	93.254	43.393	8.758	1.00 20.95	D
ATOM	4083	CE	LYS D 140	93.833	43.195	7.377	1.00 18.23	D
ATOM	4084	NZ	LYS D 140	93.743	44.457	6.617	1.00 20.40	D
MOTA	4085	С	LYS D 140	90.660	39.339	9.068	1.00 19.16	D
MOTA	4086	0	LYS D 140	91.091	38.217	9.312	1.00 19.77 1.00 21.60	D D
ATOM	4087	N	SER D 141	89.670	39.552	8.207 7.507	1.00 21.80	D
ATOM	4088	CA	SER D 141	89.030 87.859	38.438 38.948	6.653	1.00 24.88	D
ATOM	4089 4090	CB	SER D 141 SER D 141	88.288	39.858	5.655	1.00 28.69	D
MOTA	4091	OG C	SER D 141	89.989	37.605	6.636	1,00 23.26	D
ATOM ATOM	4092	Ö	SER D 141	89.692	36.454	6.327	1.00 23.33	D
ATOM	4093	N	ASP D 142	91.137	38.159	6.251	1.00 21.38	D
MOTA	4094	CA	ASP D 142	92.075	37.387	5.429	1.00 22.54	D
ATOM	4095	CB	ASP D 142	92.834	38.303	4.466	1.00 25.84	D
ATOM	4096	CG	ASP D 142	93.943	39.064	5.143	1.00 29.78	D
MOTA	4097		ASP D 142	93.760	39.486	6.309	1.00 31.16	D
MOTA	4098		ASP D 142	94.997	39.246	4.500	1.00 34.64	D D
MOTA	4099	C	ASP D 142	93.045	36.637	6.336 5.883	1.00 22.89 1.00 20.54	ם
MOTA	4100	0	ASP D 142	94.027	36.037 36.700	7.632	1.00 20.54	ם
MOTA	4101	N CA	HIS D 143 HIS D 143	92.753 93.522	36.020	8.659	1.00 19.58	D
ATOM. ATOM	4102 4103	CB	HIS D 143	93.628	34.534	8.317	1.00 19.03	D
ATOM	4104	CG	HIS D 143	92.295	33.892	8.104	1.00 23.00	D
ATOM	4105		HIS D 143	91.827	33.108	7.104	1.00 24.78	D
MOTA	4106	ND1	HIS D 143	91.237	34.087	8.967	1.00 21.97	D
ATOM	4107	CE1	HIS D 143	90.174	33.455	8.505	1.00 24.67	D
MOTA	4108		HIS D 143	90.504	32.853	7.375	1.00 24.72	D D
ATOM	4109	C	HIS D 143	94.878	36.602 35.962	8.986 9.654	1.00 20.11 1.00 21.09	D
MOTA	4110	0	HIS D 143 SER D 144	95.691 95.118	37.820	8.514	1.00 21.24	D
MOTA	4111	N CA	SER D 144	96.352	38.525	8.826	1.00 21.79	D
ATOM ATOM	4112 4113	CB	SER D 144	96.834	39.353	7.627	1.00 20.33	D
MOTA	4114	OG	SER D 144	96.047	40.511	7.434	1.00 24.32	D
ATOM	4115	c	SER D 144	95.940	39.440	9.990	1.00 21.43	D
ATOM	4116	0	SER D 144	94.830	39.317	10.504	1.00 20.74	D
MOTA	4117	N	PHE D 145	96.809	40.352	10.412	1.00 21.56	D
MOTA	4118	CA	PHE D 145	96.463	41.235	11.523	1.00 22.54	D
MOTA	4119	CB	PHE D 145		40.791	12.817	1.00 22.63 1.00 25.73	D
MOTA	4120	CG	PHE D 145		39.368	13.200 12.562	1.00 25.73	D D
MOTA	4121		PHE D 145		38.329 39.063	14.207	1.00 23.65	D
ATOM	4122		PHE D 145		37.004	12.921	1.00 27.30	D
MOTA	4123 4124		PHE D 145		37.746	14.572	1.00 25.43	D
ATOM MOTA	4125	CZ	PHE D 145		36.713	13.926	1.00 24.90	D
MOTA	4126	c	PHE D 145		42.687	11.299	1.00 22.51	D
ATOM	4127	ō	PHE D 149		43.028	10.339		D
ATOM	4128	N	PHE D 146	96.371	43.540	12.198		D
ATOM	4129	CÁ	PHE D 146			12.190		D
MOTA	4130		PHE D 146					D
MOTA	4131	CG	PHE D 146					ם ם
MOTA	4132		1 PHE D 146			12.948 11.976		D
MOTA	4133		2 PHE D 146 1 PHE D 146	93.321 92.961				D
MOTA	4134	CE	2 PHE D 146	92.981				D
MOTA MOTA	4135 4136		PHE D 140					D
ATOM	4137		PHE D 14				1.00 19.66	D
ATOM	4138		PHE D 14	96.373		14.551		D
MOTA	4139		LYS D 14	97.666	46.379	13.901	1.00 20.23	D

ATOM	4140	CA	LYS D 147	97.910	46.817	15.260	1.00 19.84	D
ATOM	4141	СВ	LYS D 147	99.184	46.148	15.796	1.00 21.50	D
ATOM	4142	CG	LYS D 147	99.651	46.679	17.134	1.00 24.87	D
MOTA	4143	CD	LYS D 147	100.764	45.832	17.724	1.00 27.18	D
ATOM	4144	CE	LYS D 147	100.220	44.515	18.253	1.00 31.41	D
MOTA	4145	NZ	LYS D 147	101.086	43.984	19.341	1.00 32.97 1.00 18.69	D D
ATOM	4146	C	LYS D 147	98.038	48.324 48.914	15.274 14.352	1.00 20.14	D
MOTA	4147	0	LYS D 147 ILE D 148	98.603 97.497	48.944	16.314	1.00 18.22	D
ATOM ATOM	4148 4149	N CA	ILE D 148	97.530	50.387	16.446	1.00 18.25	D
ATOM	4150	CB	ILE D 148	96.092	50.942	16.548	1.00 20.80	D
ATOM	4151	CG2		96.113	52.459	16.659	1.00 22.44	D
ATOM	4152	CG1		95.308	50.533	15.292	1.00 23.89	D
MOTA	4153	CD1		93.840	50.858	15.314	1.00 24.42	D
ATOM	4154	C	ILE D 148	98.369	50.816	17.646	1.00 19.71	D
MOTA	4155	0	ILE D 148	98.213	50.294	18.757	1.00 17.77	D
MOTA	4156	N	SER D 149	99.284	51.753	17.395	1.00 19.08	D
ATOM	4157	CA	SER D 149	100.173	52.278	18.424	1.00 18.19	D D
MOTA	4158	СВ	SER D 149	101.633	52.137 52.492	17.991 19.040	1.00 18.51 1.00 19.49	D
MOTA	4159	C	SER D 149 SER D 149	102.518 99.839	53.744	18.646	1.00 18.14	D
MOTA MOTA	4160 4161	0	SER D 149	99.591	54.490	17.693	1.00 18.17	D
MOTA	4162	И	TYR D 150	99.843	54.155	19.905	1.00 16.95	D
ATOM	4163	CA	TYR D 150	99.503	55.524	20.261	1.00 16.12	D
ATOM	4164	CB	TYR D 150	98.310	55.524	21.213	1.00 15.57	D
ATOM	4165	CG	TYR D 150	97.116	54.750	20.701	1.00 16.81	D
ATOM	4166	CD1	TYR D 150	96.291	55.276	19.709	1.00 14.33	D
MOTA	4167		TYR D 150	95.197	54.554	19.222	1.00 17.50	D
MOTA	4168	CD2		96.819	53.486	21.199	1.00 15.90	D
ATOM	4169	CE2		95.731	52.760	20.719	1.00 18.41 1.00 16.27	D D
MOTA	4170	CZ	TYR D 150	94.928 93.868	53.297 52.574	19.732 19.244	1.00 20.03	D
MOTA	4171 4172	C	TYR D 150 TYR D 150	100.650	56.266	20.922	1.00 16.35	D
ATOM ATOM	4172	Ö	TYR D 150	101.438	55.690	21.669	1.00 16.95	D
ATOM	4174	N	LEU D 151	100.732	57.558	20.643	1.00 16.64	D
ATOM	4175	CA	LEU D 151	101.760	58.396	21.227	1.00 16.50	D
ATOM	4176	CB	LEU D 151	102.849	58.705	20.203	1.00 15.48	D
ATOM	4177	CG	LEU D 151	103.806	59.825	20.639	1.00 17.55	D
MOTA	4178		LEU D 151	104.641	59.374	21.834	1.00 16.60	D
MOTA	4179		LEU D 151	104.702	60.213	19.476	1.00 16.11 1.00 17.56	D D
MOTA	4180	C	LEU D 151 LEU D 151	101.140 100.577	59.701 60.440	21.693 20.888	1.00 17.18	D
MOTA	4181 4182	O N	THR D 152	101.233	59.997	22.983	1.00 16.14	D
ATOM ATOM	4183	CA	THR D 152	100.690	61.259	23.448	1.00 19.47	D
ATOM	4184	CB	THR D 152	100.359	61.248	24.966	1.00 21.24	D
ATOM	4185		THR D 152	101.517	60.871	25.725	1.00 25.03	D
ATOM	4186	CG2	THR D 152	99.214	60.281	25.247	1.00 20.79	D
ATOM	4187	C	THR D 152	101.717	62.345	23.151	1.00 19.82	D
MOTA	4188	0	THR D 152	102.921	62.113	23.218	1.00 21.31	D
MOTA	4189	N	LEU D 153	101.241	63.523	22.781	1.00 20.76	D D
MOTA	4190	CA	LEU D 153	102.143	64.617 64.450	22.488 21.089	1.00 24.15 1.00 25.45	D
MOTA	4191	CB	LEU D 153	102.760 101.959	64.575	19.785	1.00 27.17	D
MOTA MOTA	4192 4193	CG	LEU D 153 L LEU D 153	100.520	64.101	19.986	1.00 27.83	D
MOTA	4194		2 LEU D 153	101.982	66.015	19.319	1.00 27.38	D
ATOM	4195	C	LEU D 153	101.440	65.952	22.601	1.00 25.73	D
ATOM	4196	ō	LEU D 153	100.208	66.028	22.681	1.00 26.55	D
ATOM	4197	N	LEU D 154	102.251	67.000	22.640	1.00 26.77	D
ATOM	4198	CA	LEU D 154	101.781	68.369	22.734	1.00 26.34	D
MOTA	4199	CB	LEU D 154	102.298	69.027	24.019	1.00 25.08	D
MOTA	4200	CG	LEU D 154	101.877	70.478		1.00 26.28	D D
ATOM	4201		1 LEU D 154	100.377	70.531	24.570	1.00 24.44 1.00 23.08	ם
MOTA	4202		LEU D 154	102.667 102.374	71.031 69.063	_	1.00 28.41	D
ATOM	4203	0	LEU D 154	102.574	69.327		1.00 27.19	D
MOTA MOTA	4204 4205	И	PRO D 155	101.534	69.351		1.00 30.32	D
MOTA	4205	CD		100.109	68.979	_	1.00 30.25	D
MOTA	4207	CA		101.965	70.014	19.294	1.00 31.71	D
ATOM	4208	CB		100.667	70.160			D
ATOM	4209	CG		99.861				D
MOTA	4210		PRO D 155	102.663	71.354			D
ATOM	4211		PRO D 155	102.110				ם מ
MOTA	4212		SER D 156	103.893				D
MOTA	4213	CA	SER D 156	104.706	16.043	22.003	2.00 10.01	_

ATOM	4214	CB	SER D	156	105.819	72.492	20.121	1.00 43.03	D
ATOM	4215	OG	SER D	156	105.288	72.385	21.430	1.00 45.30	D
ATOM	4216	C	SER D		105.311	72.763	17.694	1.00 46.03	D
		ō	SER D		104.875	72.084	16.770	1.00 47.06	D
ATOM	4217								
MOTA	4218	N	ALA D		106.316	73.609	17.534	1.00 49.61	D
MOTA	4219	CA	ALA D	157	106.931	73.756	16.222	1.00 51.03	D
MOTA	4220	CB	ALA D	157	106.977	75.231	15.828	1.00 51.20	D
ATOM	4221	C	ALA D	157	108.334	73.163	16.195	1.00 51.50	ם
ATOM	4222	0	ALA D	157	108.985	73.147	15.150	1.00 52.20	ם
ATOM	4223	N	GLU D		108.797	72.669	17.339	1.00 52.37	D
ATOM	4224	CA	GLU D		110.141	72.103	17.411	1.00 53.43	ם
								1.00 57.17	D
MOTA	4225	CB	GLO D		110.946	72.785	18.524		
ATOM	4226	CG	GLU D		110.401	72.570	19.934	1.00 61.50	a
MOTA	4227	æ	GTA D		109.278	73.529	20.291	1.00 63.75	D
MOTA	422B	OE1	GLU D	158	108.757	73.431	21.425	1.00 63.56	D
MOTA	4229	OE2	GLU D	158	108.922	74.381	19.445	1.00 65.17	D
ATOM	4230	C	GLU D	158	110.190	70.592	17.614	1.00 51.03	D
ATOM	4231	0	GLU D		111.103	70.084	18.265	1.00 51.07	D
ATOM	4232	N	GLU D		109.219	69.876	17.057	1.00 47.47	D
			GLU D		109.185	68.425	17.193	1.00 46.22	D
ATOM	4233	CA							
MOTA	4234	CB	GLU D		108.337	68.013	18.406	1.00 47.11	D
MOTA	4235	CG	GLU D	159	109.127	67.692	19.671	1.00 48.53	D
MOTA	4236	CD	GLU D	159	108.268	67.042	20.751	1.00 50.37	D
ATOM	4237	OE1	GLU D	159	107.319	67.694	21.238	1.00 50.39	Ø
ATOM	4238	OE2	GLU D	159	108.537	65.873	21.112	1.00 50.03	D
MOTA	4239	C	GLU D		108.641	67.714	15.960	1.00 43.84	D
			GLU D		107.515	67.974	15.535	1.00 44.12	D
ATOM	4240	0						1.00 39.56	D
MOTA	4241	N	SER D		109.443	66.825	15.380		
MOTA	4242	CA	ser d		108.993	66.054	14.229	1.00 37.29	D
ATOM	4243	CB	SER D	160	109.971	66.172	13.055	1.00 37.41	D
MOTA	4244	OG	SER D	160	111.070	65.298	13.206	1.00 41.72	D
ATOM	4245	C	SER D	160	108.933	64.615	14.734	1.00 35.08	D
ATOM	4246	ō	SER D		109.754	64.207	15.557	1.00 33.66	D
	4247	N	TYR D		107.961	63.846	14.260	1.00 32.11	D
ATOM							14.728	1.00 29.69	D
ATOM	4248	CA	TYR D		107.828	62.478			
ATOM	4249	CB	TYR D		106.550	62.315	15.547	1.00 29.62	D
ATOM	4250	CG	TYR D	161	106.347	63.349	16.620	1.00 29.33	D
ATOM	4251	CD1	TYR D	161	105.761	64.577	16.327	1.00 31.31	D
MOTA	4252	CE1	TYR D	161	105.513	65.515	17.329	1.00 32.70	D
ATOM	4253		TYR D		106.695	63.085	17.937	1.00 30.13	D
ATOM	4254	CE2			106.457	64.013	18.947	1.00 30.43	D
					105.863	65.223	18.638	1.00 31.92	D
ATOM	4255	CZ	TYR D					1.00 35.12	D
MOTA	4256	OH	TYR D		105.592	66.128	19.643		
MOTA	4257	C	TYR D		107.820	61.441	13.627	1.00 29.60	D
MOTA	4258	0	TYR D	161	107.493	61.728	12.473	1.00 29.45	D
MOTA	4259	N	ASP D	162	108.172	60.221	14.005	1.00 29.35	D
ATOM	4260	CA	ASP D	162	108,201	59.109	13.075	1.00 30.15	D
ATOM	4261	CB	ASP D		109.618	58.863	12.548	1.00 34.90	D
	4262	CG	ASP D		110.154	60.016	11.733	1.00 37.70	D
MOTA							10.597	1.00 40.13	D
ATOM	4263		ASP I		109.669	60.218			
MOTA	4264	OD2	ASP I		111.061	60.716	12.235	1.00 38.68	D
ATOM	4265	C	ASP D	162	107.759	57.851	13.784	1.00 29.84	D
MOTA	4266	0	ASP D	162	108.010	57.672	14.978	1.00 26.72	D
ATOM	4267	N	CYS I	163	107.088	56.984	13.039	1.00 29.31	D
ATOM	4268	CA	CYS I		106.684	55.700	13.569	1.00 29.59	D
		C	CYS		107.689	54.769	12.902	1.00 28.04	D
MOTA	4269					54.772	11.685	1.00 26.22	D
MOTA	4270	0	CYS I		107.822				
MOTA	4271	CB	CYS I		105.265	55.326	13.134	1.00 29.11	D
MOTA	4272	SG	CYS I	163	104.703	53.760	13.878	1.00 34.32	D
ATOM	4273	N	LYS I	164	108.417	54.001	13.699	1.00 29.03	D
ATOM	4274	CA	LYS I	164	109.404	53.072	13.161	1.00 29.67	D
MOTA	4275	CB	LYS I		110.730	53.238	13.911	1.00 32.54	D
ATOM		CG	LYS I		111.874	52.352	13.416	1.00 34.76	D
	4276		LYS I			52.528	14.297	1.00 34.79	D
MOTA	4277	CD			113.109			1.00 38.29	
ATOM	4278	CE		164	114.254	51.630	13.850		D
MOTA	4279	NZ		D 164	115.425	51.702	14.775	1.00 36.58	D
MOTA	4280	C	LYS I	D 164	108.863	51.651	13.322	1.00 28.94	D
ATOM	4281	0	LYS I	164	108.642	51.189	14.443	1.00 29.32	D
ATOM	4282	N		0 165	108.632	50.974	12.197	1.00 27.33	D
ATOM	4283	CA		D 165	108.100	49.618	12.212	1.00 26.58	Ø
		CB		D 165	106.797	49.516	11.359	1.00 27.12	D
MOTA	4284					48.122	11.462	1.00 25.56	D
MOTA	4285		L VAL I		106.199				D
MOTA	4286		VAL I		105.787	50.544	11.827	1.00 27.97	
MOTA	4287	C	VAL	D 165	109.113	48.600	11.690	1.00 26.91	D

		_	D 16F	109.621	48.720	10.583	1.00 25.56	D
ATOM	4288	0	VAL D 165				1.00 28.75	Ď
MOTA	4289	N	GLU D 166	109.414	47.606	12.513		
MOTA	4290	CA	GLU D 166	110.338	46.544	12.139	1.00 30.67	D
MOTA	4291	CB	GLU D 166	111.445	46.410	13.194	1.00 33.57	ם
MOTA	4292	CG	GLU D 166	112.452	47.565	13.142	1.00 41.68	D
ATOM	4293	CD	GLU D 166	113.506	47.526	14.244	1.00 46.12	D
	4294		GLU D 166	114.482	48.304	14.146	1.00 49.01	D
MOTA					46.736	15.206	1.00 49.40	D
MOTA	4295		GLU D 166	113.363				
MOTA	4296	C	GLU D 166	109.543	45.243	12.008	1.00 30.18	D
ATOM	4297	0	GLU D 166	108.737	44.900	12.878	1.00 28.51	D
ATOM	4298	N	HIS D 167	109.759	44.535	10.907	1.00 29.48	D
ATOM	4299	CA	HIS D 167	109.056	43.281	10.648	1.00 30.29	D
		CB	HIS D 167	107.686	43.569	10.025	1.00 29.56	D
MOTA	4300					9.903	1.00 30.02	D
MOTA	4301	CG	HIS D 167	106.808	42.363			Ď
MOTA	4302		HIS D 167	106.562	41.541	8.856	1.00 29.91	
ATOM	4303	ND1	HIS D 167	106.068	41.871	10.957	1.00 31.27	D
MOTA	4304	CEL	HIS D 167	105.404	40.798	10.564	1.00 28.43	D
ATOM	4305		HIS D 167	105.687	40.576	9.293	1.00 28.97	D
	4306	c	HIS D 167	109.886	42.440	9.684	1.00 30.36	D
ATOM				110.607	42.976	8.842	1.00 30.66	D
MOTA	4307	0	HIS D 167				1.00 31.13	D
MOTA	4308	N	TRP D 168	109.775	41.122	9.801		
MOTA	4309	CA	TRP D 168	110.521	40.219	8.930	1.00 32.08	D
ATOM	4310	CB	TRP D 168	110.270	38.765	9.336	1.00 28.28	D
ATOM	4311	CG	TRP D 168	110.665	38.475	10.739	1.00 26.36	D
ATOM	4312		TRP D 168	110.031	37.556	11.635	1.00 25.51	D
ATOM	4313	CB2		110.759	37.578	12.842	1.00 26.35	D
				108.916	36.715	11.534	1.00 24.88	D
MOTA	4314	CE3			39.004	11.416	1.00 27.27	D
MOTA	4315		TRP D 168	111.721				D
MOTA	4316		TRP D 168	111.786	38.471	12.682	1.00 28.25	
ATOM	4317	CZ2	TRP D 168	110.412	36.791	13.943	1.00 27.00	D
ATOM	4318	CZ3	TRP D 168	108.568	35.932	12.628	1.00 25.90	D
ATOM	4319	CH2		109.315	35.976	13.817	1.00 26.65	D
ATOM	4320	C	TRP D 168	110.180	40.403	7.452	1.00 33.22	D
			TRP D 168	111.011	40.139	6.582	1.00 33.90	D
MOTA	4321	0			40.853	7.174	1.00 34.75	D
MOTA	4322	N	GLY D 169	108.959				D
MOTA	4323	CA	GLY D 169	108.533	41.060	5.797	1.00 36.14	
ATOM	4324	C	GLY D 169	109.056	42.359	5.215	1.00 37.80	D
ATOM	4325	0	GLY D 169	108.635	42.796	4.139	1.00 36.95	D
MOTA	4326	N	LEU D 170	109.979	42.981	5.938	1.00 38.89	D
	4327	CA	LEU D 170	110.578	44.234	5.509	1.00 40.79	D
MOTA			LEU D 170	110.212	45.356	6.480	1.00 39.77	D
ATOM	4328	CB			45.765	6.581	1.00 39.57	D
MOTA	4329	CG	LEU D 170	108.745				D
ATOM	4330	CD:	L LEU D 170	108.592	46.809	7.671	1.00 38.10	
ATOM	4331	CD2	LEU D 170	108.267	46.308	5.243	1.00 39.58	D
ATOM	4332	C	LEU D 170	112.092	44.085	5.465	1.00 42.12	D
	4333	0	LEU D 170	112.688	43.506	6.370	1.00 41.54	D
ATOM	4334	N	ASP D 171	112.706	44.613	4.411	1.00 45.36	D
				114.158	44.559	4.252	1.00 48.35	D
ATOM	4335	CA	ASP D 171			2.820	1.00 50.69	D
MOTA	4336	CB	ASP D 171	114.539	44.947			
MOTA	4337	CG	ASP D 171	113.467	45.775	2.137	1.00 52.75	D
ATOM	4338	OD:	1 ASP D 171	113.076	46.827	2.689	1.00 54.19	Ø
ATOM	4339	OD:	2 ASP D 171	113.012	45.372	1.046	1.00 54.32	D
MOTA	4340	C	ASP D 171	114.849	45.485	5.255	1.00 48.43	D
		ŏ	ASP D 171	115.816	45.090	5.910	1.00 48.29	D
MOTA	4341				46.715	5.364	1.00 48.92	D
MOTA	4342	N	LYS D 172	114.348			1.00 49.86	D
MOTA	4343	CA		114.883	47.707			
ATOM	4344	CB	LYS D 172	115.502	48.898		1.00 51.58	D
MOTA	4345	CG	LYS D 172	116.667	48.566		1.00 55.86	D
MOTA	4346	CD	LYS D 172	116.203	47.963	3.316		ם
ATOM	4347			115.408	48.966	2.493	1.00 59.62	D
	4348			114.946	48.368	1.211	1.00 59.53	D
ATOM				113.734	48.224			D
ATOM	4349		LYS D 172					D
MOTA	4350		LYS D 172	112.564	48.026			ā
ATOM	4351	N	PRO D 173	114.050				
ATOM	4352	CD	PRO D 173	115.355				D
MOTA	4353		PRO D 173	112.974	49.400			D
MOTA	4354			113.722		10.305	1.00 44.19	D
ATOM	4355			114.950			1.00 45.63	D
			PRO D 173	112.180				D
MOTA	4356							D
ATOM	4357		PRO D 173	112.746				D
MOTA	4358		LEU D 174	110.869				D
MOTA	4359	CZA		110.023				
ATOM	4360	CE	LEU D 174	108.675				D
ATOM	4361		LEU D 174	107.900	51.223	6.303	1.00 40.55	D

ATOM	4362	CD1	TEA D	174	106.637	50.397	6.151	1.00 42.25	D
ATOM	4363		TEA D		107.568	52.698	6.448	1.00 42.67	D
MOTA	4364	c	LEU D		109.845	52.586	8.753	1.00 39.80	D
ATOM	4365	ō	TEG D		109.645	52.420	9.955	1.00 39.99	ם
		N	TEO D		109.947	53.792	8.200	1.00 38.49	Ď
ATOM	4366	CA	TEO D		109.787	55.016	8.983	1.00 38.04	D
ATOM	4367		FEO D		111.095	55.812	9.045	1.00 38.62	D
ATOM	4368	CB				55.442	10.113	1.00 38.70	D D
ATOM	4369	CG	TEO D		112.127			1.00 39.24	D
ATOM	4370		FEQ D		111.518	55.648	11.489		D
ATOM	4371		TEO D		112.577	54.001	9.936	1.00 40.07	
MOTA	4372	С	TEO D		108.712	55.892	8.372	1.00 37.31	D
MOTA	4373	0	LEU D		108.885	56.432	7.282	1.00 38.54	ם
MOTA	4374	N	LYS D		107.599	56.033	9.076	1.00 35.14	D
MOTA	4375	CA	LYS D	176	106.511	56.850	8.577	1.00 34.26	D
ATOM	4376	CB	LYS D	176	105.175	56.124	8.768	1.00 33.88	D
ATOM	4377	CG	LYS D	176	104.204	56.325	7.620	1.00 36.72	ם
MOTA	4378	CD	LYS D	176	104.829	55.887	6.295	1.00 37.68	D
ATOM	4379	CE	LYS D	176	103.820	55.913	5.155	1.00 39.32	D
ATOM	4380	NZ	LYS D		103.195	57.254	4.974	1.00 40.75	D
MOTA	4381	C	LYS D		106.523	58.166	9.335	1.00 32.22	D
MOTA	4382	ō	LYS D		106.272	58.204	10.537	1.00 32.35	D
ATOM	4383	N	HIS D		106.825	59.243	8.625	1.00 29.85	D
ATOM	4384	CA	HIS D		106.897	60.563	9.229	1.00 29.87	D
			HIS D		107.836	61.456	8.411	1.00 30.84	D
ATOM	4385	CB	HIS D		108.014	62.830	8.979	1.00 31.41	D
ATOM	4386	CG					8.529	1.00 32.01	D
MOTA	4387		HIS D		107.607	64.042		1.00 32.16	D
MOTA	4388		HIS D		108.695	63.067	10.155 10.402	1.00 32.10	D
ATOM	4389		HIS D		108.704	64.365			D
MOTA	4390		HIS D		108.051	64.979	9.431	1.00 31.08	D
MOTA	4391	C	HIS D		105.532	61.228	9.332	1.00 29.28	
MOTA	4392	0	HIS D		104.709	61.121	8.429	1.00 27.97	D
MOTA	4393	N	TRP D		105.295	61.922	10.439	1.00 29.05	D
ATOM	4394	CA	TRP D	178	104.031	62.617	10.619	1.00 29.38	D
ATOM	4395	CB	TRP D	178	103.518	62.464	12.048	1.00 26.73	D
ATOM	4396	CG	TRP D	178	102.205	63.165	12.243	1.00 27.32	D
ATOM	4397	CD2	TRP D	178	101.939	64.262	13.122	1.00 24.87	D
ATOM	4398	CE2	TRP D	178	100.580	64.608	12.959	1.00 26.97	D
ATOM	4399	CE3	TRP D	178	102.714	64.986	14.033	1.00 26.15	D
MOTA	4400	CD1	TRP D	178	101.028	62.898	11.599	1.00 26.41	D
MOTA	4401	NE1	TRP D	178	100.050	63.759	12.023	1.00 25.31	D
ATOM	4402		TRP D		99.980	65.649	13.675	1.00 25.60	D
ATOM	4403	CZ3			102.118	66.021	14.746	1.00 27.98	D
MOTA	4404		TRP D		100.763	66.340	14.562	1.00 27.02	D
ATOM	4405	C	TRP D		104.185	64.100	10.294	1.00 30.33	D
		Ö	TRP D		104.756	64.824	11.143	1.00 29.85	D
ATOM	4406		TRPD		103.745	64.512	9.193	1.00 32.23	D
ATOM	4407				113.641	35.776	8.019	1.00 59.19	E
ATOM	4408	CB	SER E			35.748	8.608	1.00 59.65	E
MOTA	4409	OG	SER E		112.349			1.00 57.92	E
MOTA	4410	С	SER E		114.352	33.977	9.601	1.00 57.45	E
MOTA	4411	0	SER E		114.571	32.945	8.970		
MOTA	4412	N	SER E		116.055	35.305	8.352	1.00 59.31	E
MOTA	4413	CA	SER E	3	114.719	35.342	9.020	1.00 58.85	E
MOTA	4414	N	PRO E		113.799	33.958	10.824	1.00 56.65	E
MOTA	4415	CD	PRO E	4	113.679	35.092	11.759	1.00 56.20	E
ATOM	4416	CA	PRO E	4	113.403	32.704	11.472	1.00 55.50	B
MOTA	4417	CB	PRO E	4	113.362	33.086	12.946	1.00 56.49	E
MOTA	4418	CG	PRO E	4	112.870	34.493	12.893	1.00 56.56	E
ATOM	4419	C	PRO E	4	112.046	32.217	10.957	1.00 53.68	E
ATOM	4420	0	PRO E	4	111.168	33.024	10.648	1.00 54.06	E
MOTA	4421	N	GLU E	5	111.875	30.903	10.855	1.00 51.52	E
MOTA	4422	CA	GLU E	5	110.610	30.360	10.373	1.00 49.69	E
ATOM	4423	СВ	GLU E		110.831	29.007	9.676	1.00 53.42	B
ATOM	4424	CG	GLU E		111.305	27.867	10.561	1.00 57.99	E
MOTA	4425	CD	GLU E		111.671	26.626	9.758	1.00 60.86	E
MOTA	4426		1 GLU E		110.857	26.196	8.908	1.00 62.41	E
ATOM	4427		2 GLU E		112.772	26.077	9.979	1.00 63.42	В
	4428	C C	GLU E		109.619	30.231	11.525	1.00 45.48	E
MOTA	4428		GLU E		109.919	29.644	12.564	1.00 46.07	E
MOTA		O N			109.919	30.800	11.337	1.00 40.87	E
ATOM	4430	N	ASP I			30.782	12.363	1.00 36.20	E
MOTA	4431				107.403	32.214	12.503	1.00 35.53	E
MOTA	4432				106.911	32.323	13.827	1.00 33.60	B
MOTA	4433				105.995			1.00 34.88	E
ATOM	4434		1 ASP I		105.185	33.268			E
MOTA	4435	OD:	2 ASP I	E 6	106.089	31.487		1.00 33.84	
							2		

ATOM	4436	C	ASP	E	6	106.229	29.915	11.938	1.00 33.07	E
MOTA	4437	0	ASP	E	6	105.882	29.867	10.762	1.00 32.95	E
ATOM	4438	N	PHE		7	105.632	29.228	12.906	1.00 31.08	E
	4439	CA	PHE		7	104.466	28.380	12.669	1.00 29.18	E
MOTA								13.116	1.00 31.11	B
ATOM	4440	CB	PHE		7	104.760	26.950			
ATOM	4441	CG	PHE		7	105.833	26.278	12.305	1.00 31.97	E
ATOM	4442	CD1	PHE	E	7	105.544	25.745	11.053	1.00 31.67	Ε
ATOM	4443	CD2	PHE	E	7	107.141	26.200	12.782	1.00 32.49	E
ATOM	4444		PHE		7	106.546	25.141	10.282	1.00 33.41	E
					7	108.148	25.602	12.023	1.00 32.29	E
ATOM	4445	CE2								
MOTA	4446	CZ	PHE	E	7	107.850	25.071	10.770	1.00 31.62	E
ATOM	4447	C	PHE	E	7	103.345	28.994	13.504	1.00 27.19	E
ATOM	4448	0	PHE	E	7	103.483	29.151	14.715	1.00 25.77	B
MOTA	4449	N	VAL	E	8	102.238	29.340	12.855	1.00 25.52	E
MOTA	4450	CA	VAL		8	101.127	29.998	13.538	1.00 23.97	E
						100.903		12.949	1.00 22.51	E
MOTA	4451	CB	VAL		8		31.411			
MOTA	4452		VAL		8	99.789	32.130	13.703	1.00 20.58	E
ATOM	4453	CG2	VAL	E	8	102.205	32.211	13.002	1.00 22.51	B
ATOM	4454	C	VAL	E	8	99.785	29.275	13.510	1.00 24.21	B
ATOM	4455	0	VAL		8	99.369	28.736	12.485	1.00 25.26	B
					9 .	99.096	29.288	14.643	1.00 23.98	R
MOTA	4456	N	TYR							B
ATOM	4457	CA	TYR		9	97.786	28.663	14.724	1.00 23.53	
ATOM	4458	CB	TYR	E	9	97.796	27.505	15.718	1.00 24.07	B
ATOM	4459	CG	TYR	E	9	96,562	26.640	15.627	1.00 25.27	B
MOTA	4460	CD1	TYR	E	9	96.570	25.460	14.889	1.00 27.68	E
ATOM	4461		TYR		9	95.435	24.658	14.801	1.00 27.67	B
					9	95.384	27.002	16.272	1.00 24.82	E
MOTA	4462	CD2	TYR						1.00 25.29	B -
MOTA	4463	CE2	TYR		9	94.245	26.211	16.191		
ATOM	4464	\mathbf{cz}	TYR	B	9	94.277	25.040	15.458	1.00 26.82	B
MOTA	4465	OH	TYR	B	9	93.163	24.240	15.403	1.00 27.65	E
ATOM	4466	C	TYR	E	9	96.775	29.707	15.179	1.00 23.14	E
MOTA	4467	ō	TYR		9	97.037	30.476	16.106	1.00 23.66	E
						95,622	29.739	14.523	1.00 21.64	E
MOTA	4468	N	GLN		10					E
MOTA	4469	CA	GLN	E	10	94.582	30.686	14.892	1.00 21.14	
MOTA	4470	CB	GLN	E	10	94.438	31.793	13.843	1.00 20.35	B
ATOM	4471	CG	GLN	E	10	95.677	32.598	13.529	1.00 19.58	E
ATOM	4472	CD	GLN		10	95.410	33.655	12.461	1.00 18.44	E
	4473	OE1			10	94.498	34.474	12.593	1.00 19.00	B
ATOM								11.400	1.00 18.89	B
MOTA	4474	NE2			10	96.206	33.640			
MOTA	4475	C	GLN		10	93.232	29.997	15.006	1.00 19.74	E
MOTA	4476	0	GLN	E	10	92.904	29.113	14.223	1.00 21.71	E
MOTA	4477	N	PHE	B	11	92.450	30.408	15.991	1.00 19.13	E
ATOM	4478	CA	PHE	E	11	91.108	29.887	16.145	1.00 16.86	B
ATOM	4479	CB	PHE		11	90.981	28.881	17.271	1.00 16.74	E
							28.466	17.517	1.00 18.71	E
ATOM	4480	CG	PHE		11	89.562				E
MOTA	4481	CD1	PHE	E	11	88.910	27.615	16.626	1.00 21.10	
ATOM.	4482	CD2	PHE	E	11	88.849	28.985	18.595	1.00 18.11	E
ATOM	4483	CE1	PHE	E	11	87.559	27.290	16.807	1.00 22.40	E
ATOM	4484	CB2			11	87.499	28.671	18.789	1.00 15.75	E
	4485	CZ	PHE		11	86.854	27.826	17.898	1.00 21.25	E
MOTA							31.069	16.451	1.00 17.10	8
MOTA	4486	С	PHE		11	90.218				E
ATOM	4487	0	PHE		11	90.461	31.819	17.406	1.00 13.97	
MOTA	4488	N	LYS	E	12	89.197	31.241	15.622	1.00 16.07	E
MOTA	4489	CA	LYS	B	12	88.266	32.338	15.789	1.00 16.96	E
MOTA	4490	CB	LYS	E	12	88.308	33.246	14.564	1.00 17.05	В
ATOM	4491	CG	LYS		12	89.703	33.748	14.200	1.00 17.57	E
						89.663	34.535	12.888	1.00 18.92	E
MOTA	4492	CD	LYS		12		35.136	12.532	1.00 17.07	E
ATOM	4493	CE	LYS		12	91.018				
MOTA	4494	NZ	LYS		12	90.920	36.063	11.362	1.00 14.26	E
ATOM	4495	С	LYS	E	12	86.856	31.803	15.987	1.00 17.87	. В
ATOM	4496	0	LYS	E	12	86.354	31.039	15.165	1.00 16.82	E
ATOM	4497	N	GL'		13	86.235	32.195	17.098	1.00 18.19	E
						84.875	31.776	17.391	1.00 19.62	B
MOTA	4498	CA	GL		13		32.939	17.010	1.00 19.93	E
MOTA	4499	C	GL)		13	83.991				
ATOM	4500	0	GL?		13	83.539	33.695	17.868	1.00 21.65	E
ATOM	4501	N	MET	r e	14	83.728	33.070	15.715	1.00 19.89	E
ATOM	4502	CA	ME?		14	82.947	34.184	15.197	1.00 20.54	E
ATOM	4503	СВ	ME		14	83.430		13.785	1.00 21.02	E
ATOM	4504	CG	ME'		14	84.937			1.00 23.04	B
									1.00 25.32	E
MOTA	4505	SD		E	14	85.587			1.00 20.32	E
MOTA	4506			r e	14	85.218				
MOTA	4507			r e	14	81.429			1.00 20.83	E
ATOM	4508	0	ME'	r e	14	80.859			1.00 20.77	E
MOTA	4509			SE	15	80.789		15.377	1.00 20.66	E

MOTA	4510	CA	CYS	B	15	79.332	35.336	15.418	1.00 22.09	E
MOTA	4511	C	CYS		15	78.882	36.495	14.524	1.00 21.39	E
ATOM	4512	0	CYS		15	79.393	37.614	14.644 16.848	1.00 19.38 1.00 22.10	e
MOTA	4513	CB SG	CYS		15 15	78.841 78.970	35.616 34.281	18.094	1.00 26.75	E
ATOM ATOM	4514 4515	N	TYR		16	77.931	36.229	13.633	1.00 20.94	E
ATOM	4516	CA	TYR		16	77.408	37.270	12.752	1.00 21.23	E
MOTA	4517	CB	TYR	E	16	77.548	36.858	11.287	1.00 18.37	E
MOTA	4518	CG	TYR		16	78.972	36.574	10.876	1.00 19.23 .	E
MOTA	4519		TYR		16	79.576	35.354 35.084	11.178 10.789	1.00 18.71 1.00 18.69	E E
ATOM	4520 4521	CD2	TYR TYR		16 16	80.875 79.715	37.524	10.78	1.00 20.25	B
ATOM ATOM	4522	CE2	TYR		16	81.022	37.270	9.785	1.00 17.18	E
ATOM	4523	CZ	TYR		16	81.595	36.047	10.088	1.00 21.03	E
ATOM	4524	OH	TYR		16	82.872	35.775	9.662	1.00 22.99	E
MOTA	4525	C	TYR		16	75.938 75.132	37.543 36.612	13.085 13.199	1.00 22.17 1.00 21.71	e
ATOM ATOM	4526 4527	N O	TYR		16 17	75.607	38.825	13.247	1.00 23.05	E
ATOM	4528	CA	PHE		17	74.254	39.263	13.591	1.00 23.67	B
ATOM	4529	СВ	PHE		17	74.261	39.988.	14.942	1.00 22.49	E
ATOM	4530	CG	PHE		17	74.813	39.172	16.084	1.00 25.10	E
MOTA	4531		PHE		17	74.007	38.270	16.772	1.00 24.22	E
ATOM	4532		PHE		17 17	76.140 74.516	39.318 37.526	16.482 17.844	1.00 24.67 1.00 24.68	E
ATOM ATOM	4533 4534	CE2			17	76.656	38.579	17.548	1.00 24.45	B
ATOM	4535	CZ	PHE		17	75.843	37.684	18.228	1.00 24.13	E
ATOM	4536	С	PHE	E	17	73.673	40.223	12.549	1.00 25.10	E
ATOM	4537	0	PHE		17	74.390	41.034	11.971	1.00 24.65	E
ATOM	4538	N	THR		18	72.365 71.638	40.122 40.983	12.333 11.405	1.00 27.15 1.00 29.69	e
ATOM ATOM	4539 4540	CA CB	THR		18 18	71.638	40.383	9.978	1.00 29.46	E
ATOM	4541		THR		18	72.949	40.252	9.500	1.00 32.31	E
ATOM	4542	CG2	THR	E	18	70.863	41.321	9.032	1.00 28.09	E
MOTA	4543	С	THR		18	70.217	41.080	11.950	1.00 31.56	E
MOTA	4544	0	THR		18	69.638	40.071	12.355 11.969	1.00 32.09 1.00 33.38	E
ATOM	4545	N	asn asn		19 19	69.661 68.316	42.290 42.495	12.497	1.00 35.02	E
ATOM ATOM	4546 4547	CA CB	ASN		19	67.279	41.755	11.647	1.00 37.99	E
ATOM	4548	CG	ASN		19	66.779	42.587	10.489	1.00 42.21	E
ATOM	4549	OD1	ASN	E	19	66.271	43.695	10.687	1.00 47.70	E
MOTA	4550		ASN		19	66.910	42.063	9.273	1.00 43.13	B E
ATOM	4551	C	ASN		19 19	68.264 67.487	41.977 41.077	13.924 14.233	1.00 34.10 1.00 34.27	E
ATOM ATOM	4552 4553	и О	ASN GLY		20	69.088	42.553	14.795	1.00 33.50	B
ATOM	4554	CA	GLY		20	69.120	42.106	16.175	1.00 33.61	E
ATOM	4555,	C	GLY	E	20	69.575	40.663	16.175	1.00 33.98	E
MOTA	4556	0	GLY		20	70.580	40.343	15.541	1.00 34.56 1.00 34.08	e
ATOM	4557	N	THE		21 21	68.847 69.198	39.789 38.372	16.866 16.897	1.00 35.71	E
MOTA MOTA	4558 4559	CA CB	THE		21	69.193	37.809	18.335	1.00 37.69	E
ATOM	4560		L THE		21	67.907	38.026	18.930	1.00 39.78	E
ATOM	4561	CG:	THE	RE	21	70.268	38.480	19.174	1.00 38.05	E
MOTA	4562	C		R	21	68.251	37.517	16.050	1.00 35.19	E
ATOM	4563	0		RE	21	68.092 67.619	36.324 38.129	16.303 15.052	1.00 36.08 1.00 34.15	E
ATOM ATOM	4564 4565	N CA		JE Je	22 22	66.705	37.405	14.176	1.00 34.08	E
ATOM	4566	СВ		JE	22	65.868	38.388	13.354	1.00 33.12	E
ATOM	4567	CG		UE	22	64.781	39.073	14.164	1.00 33.66	E
MOTA	4568	æ		UE	22	64.173	40.266	13.451	1.00 35.85	e
MOTA	4569		1 GL			63.865	40.151 41.317	12.244 14.105	1.00 35.10 1.00 38.34	E
MOTA	4570		2 GL	UE		63.995 67.523	36.503	13.265	1.00 33.80	E
MOTA MOTA	4571 4572	0		UE		67.205	35.329	13.092	1.00 34.50	E
MOTA	4573	N		G E		68.574	37.065	12.678	1.00 33.59	E
MOTA	4574	CA	AR	G E		69.467	36.298	11.818	1.00 33.75	E
MOTA	4575	CB		G E		69.703	36.996	10.470	1.00 36.33 1.00 42.06	E
MOTA	4576			G E G E		68.599 67.342		9.434 9.813	1.00 47.83	E
MOTA MOTA	4577 4578			GE		66.408			1.00 51.02	E
ATOM	4579			GE		65.349			1.00 52.66	E
MOTA	4580	NH	1 AR	G E	23	65.087				Ē
MOTA	4581			G E		64.555				E
ATOM	4582			G E		70.788				E
ATOM	4583	0	AR	G E	23	71.465	31.1/2	12.02/		_

									1.00 28.33	B
MOTA	4584	N	VAL		24	71.149	34.955	12.909	1.00 25.06	E
MOTA	4585	CA	VAL		24	72.394	34.735	13.621		E
MOTA	4586	ĊВ	VAL		24	72.148	34.500	15.129	1.00 22.98	E
ATOM	4587	CG1	AYP	E	24	73.456	34.106	15.817	1.00 21.05	
ATOM	4588	CG2	VAL	E	24	71.582	35.762	15.763	1.00 21.04	E
ATOM	4589	С	VAL	E	24	73.144	33.550	13.049	1.00 23.08	B
ATOM	4590	0	VAL	B	24	72.600	32.458	12.914	1.00 24.17	E
ATOM	4591	N	ARG		25	74.398	33.778	12.694	1.00 23.02	E
		CA	ARG		25	75.223	32.718	12.156	1.00 23.30	R
ATOM	4592					75.511	32.930	10.659	1.00 24.06	E
MOTA	4593	CB	ARG		25				1.00 25.99	E
ATOM	4594	CG	ARG		25	76.653	32.044	10.176		E
ATOM	4595	CD	ARG	K	25	76.470	31.478	8.774	1.00 28.29	
ATOM	4596	NE	ARG	Е	25	76.468	32.502	7.743	1.00 29.69	E
MOTA	4597	CZ	ARG	E	25	76.786	32.287	6.466	1.00 29.57	E
ATOM	4598	NH1	ARG	E	25	77.145	31.075	6.047	1.00 27.28	E
ATOM	4599		ARG		25	76.733	33.293	5.604	1.00 26.98	E
	4600	C	ARG		25	76.535	32.631	12.916	1.00 22.65	E
ATOM			ARG		25	77.261	33.620	13.041	1.00 22.47	E
ATOM	4601	0				76.828	31.444	13.433	1.00 21.04	B
MOTA	4602	N	LEU		26			14.152	1.00 21.94	E
MOTA	4603	CA	LEU		26	78.069	31.227			E
MOTA	4604	CB	TEA		26	77.834	30.338	15.383	1.00 21.37	
ATOM	4605	CG	LEU	E	26	79.054	29.778	16.128	1.00 22.89	E
ATOM	4606	CD1	LEU	E	26	78.723	29.567	17.602	1.00 25.16	E
ATOM	4607	CD2	LEU	E	26	79.483	28.466	15.493	1.00 23.51	B
	4608	c	LEU		26	79.032	30.552	13.193	1.00 21.17	E
ATOM			LEU		26	78.637	29.674	12.432	1.00 21.77	B
MOTA	4609	0					30.983	13.201	1.00 19.92	E
MOTA	4610	N	VAL		27	80.285			1.00 21.31	В
MOTA	4611	CA	VAL		27	81.278	30.358	12.345		E
MOTA	4612	CB	VAL		27	81.530	31.166	11.039	1.00 20.44	
ATOM	4613	CG1	VAL	B	27	82.524	30.420	10.156	1.00 21.63	E
ATOM	4614	CG2	VAL	E	27	80.221	31.366	10.275	1.00 20.48	E
MOTA	4615	С	VAL	E	27	82.581	30.231	13.112	1.00 21.74	E
ATOM	4616	o	VAL		27	83.189	31.228	13.487	1.00 24.11	E
		N	SER		28	82.994	29.001	13.383	1.00 20.88	B
ATOM	4617					84.249	28.799	14.084	1.00 21.53	E
MOTA	4618	CA	SER		28		27.702	15.152	1.00 20.62	E
MOTA	4619	CB	SER		28	84.113			1.00 29.22	E
MOTA	4620	OG	SER	E	28	83.693	26.475	14.598		E
ATOM	4621	C	SER	E	28	85.274	28.433	13.006	1.00 21.41	
ATOM	4622	0	SER	E	28	84.992	27.631	12.105	1.00 19.11	E
ATOM	4623	N	ARG	E	29	86.450	29.051	13.090	1.00 18.23	B
MOTA	4624	CA	ARG		29	87.496	28.838	12.105	1.00 18.45	B
		СВ	ARG		29	87.701	30.124	11.287	1.00 16.91	E
MOTA	4625		ARG		29	86.433	30.817	10.810	1.00 17.70	E
MOTA	4626	CG					32.117	10.109	1.00 18.98	E
MOTA	4627	CD	ARG		29	86.791		9.705	1.00 20.82	E
MOTA	4628	NE	ARG		29	85.631	32.902		1.00 20.02	Ē
MOTA	4629	CZ	ARG		29	84.939	32.704	8.586	_	
MOTA	4630	NH:	L ARG	E	29	85.285	31.739	7.743	1.00 21.05	E
MOTA	4631	NH:	2 ARG	E	29	83.904	33.482	8.309	1.00 20.13	E
ATOM	4632		ARG		29	88.842	28.435	12.710	1.00 18.44	E
ATOM	4633		ARG		29	89.401	29.171	13.520	1.00 19.35	E
			SER		30	89.351	27.269	12.315	1.00 18.98	E
ATOM	4634		SER			90.657	26.788	12.774	1.00 21.70	E
ATOM	4635					90.619	25.284	13.028	1.00 22.10	E
MOTA	4636		SEF					14.072	1.00 27.24	E
MOTA	4637	OG	Sef			89.718				E
MOTA	4638	C	SEF	E	30	91.637			1.00 23.03	E
MOTA	4639	0	SEF	ß	30	91.509			1.00 23.56	
MOTA	4640	N	ILE	3 B	31	92.611	27.978		1.00 23.05	E
ATOM	4641		ILI	2 E	31	93.560	28.439	10.923	1.00 22.24	E
ATOM	4642					93.563	29.997	10.856	1.00 22.84	E
			2 IL			94.163			1.00 19.19	E
MOTA	4643					92.143				E
MOTA	4644		1 ILI							E
MOTA	4645		1 IL			91.144				E
MOTA	4646	C	IL	EE		95.013		•		E
MOTA	4647	7 0	IL	E B	31	95.566			_	
MOTA	4648	3 N	TY	R E	32	95.625				E
ATOM	4645			R E		97.030	27.089	10.120		E
ATOM	4650			R E		97.277	7 25.759	9.417	1.00 26.61	E
	465			RE		98.733			1.00 29.24	E
MOTA) TY			99.423				E
ATOM	465					100.770			_	E
ATOM	465		31 TY							E
MOTA	465		2 TY			99.426				E
MOTA	465		32 TY			100.774				E
MOTA	465	6 C2	YT Y	R I	32	101.438				
MOTA	465		I TY	R I	32	102.76	8 24.28	9.522	2 1.00 33.44	E
		-								

		_		_		07 700	20 225	0 252	1.00 24.83	B
ATOM	4658	С	TYR E		32	97.700	28.225	9.353		
ATOM	4659	0	TYR I	3	32	97.444	28.415	8.164	1.00 25.49	B
MOTA	4660	N	ASN I	3	33	98.543	28.985	10.045	1.00 24.28	E
ATOM	4661	CA	ASN I	2	33	99.202	30.146	9.461	1.00 24.25	E
							29.740	8.324	1.00 23.93	E
MOTA	4662	CB	ASN I		33	100.144				E
MOTA	4663	CG	asn i	B	33	101.379	29.014	8.834	1.00 25.26	
ATOM	4664	OD1	ASN I	В	33	102.003	29.439	9.808	1.00 26.40	B
ATOM	4665	ND2	ASN I	R	33	101.737	27.918	8.181	1.00 25.47	E
					33	98.114	31.099	8.980	1.00 24.88	E
ATOM	4666	С	ASN 1							E
ATOM	4667	0	ASN 1	E	33	97.494	31.780	9.799	1.00 25.88	
MOTA	4668	N	ARG 1	Е	34	97.864	31.163	7.677	1.00 24.52	E
ATOM	4669	CA	ARG :	R	34	96.815	32.055	7.194	1.00 26.32	E
			ARG		34	97.385	33.175	6.317	1.00 26.61	E
ATOM	4670	CB						7.072	1.00 26.37	E
ATOM	4671	CG	ARG :		34	97.999	34.346			
MOTA	4672	CD	ARG :	E	34	97.776	35.646	6.304	1.00 28.18	E
ATOM	4673	NE	ARG	E	34	97.886	35.429	4.865	1.00 31.86	E
		CZ	ARG		34	97.607	36.332	3.931	1.00 33.42	E
ATOM	4674								1.00 35.40	E
ATOM	4675		ARG		34	97.197	37.550	4.265		
ATOM	4676	NH2	ARG	E	34	97.722	36.003	2.653	1.00 35.29	B
ATOM	4677	С	ARG	E	34	95.728	31.333	6.417	1.00 26.98	E
			ARG		34	94.896	31.968	5.763	1.00 28.88	E
ATOM	4678	0							1.00 26.13	B
MOTA	4679	N	GLU	E	35	95.719	30.010	6.481		
MOTA	4680	CA	GLU	B	35	94.698	29.279	5.759	1.00 27.02	E
ATOM	4681	CB	GLU	R	35	95.350	28.359	4.720	1.00 31.96	E
			GLU		35	96.284	27.301	5.278	1.00 38.52	E
ATOM	4682	CG							1.00 42.24	E
MOTA	4683	CD	GĽŪ		35	97.116	26.633	4.192		
ATOM	4684	OEL	GLU	E	35	98.180	27.187	3.832	1.00 44.86	Ē
ATOM	4685	OE2	GLU	E	35	96.699	25.565	3.690	1.00 43.70	E
		C	GLU		35	93.754	28.498	6.671	1.00 25.31	E
MOTA	4686						27.709	7.522	1.00 22.18	E
ATOM	4687	0	GLU		35	94.175				В
MOTA	4688	N	GLU	E	36	92.464	28.756	6.498	1.00 24.46	
MOTA	4689	CA	GLU	B	36	91.438	28.085	7.272	1.00 24.13	E
ATOM	4690	СВ	GLU		36	90.085	28.731	7.001	1.00 24.37	B
						88.975	28.295	7.928	1.00 25.26	E
ATOM	4691	CG	GLD		36				1.00 26.01	E
MOTA	4692	CD	GLU	E	36	87.669	28.991	7.604		
MOTA	4693	OE1	. GLU	E	36	87.672	29.847	6.694	1.00 27.25	E
MOTA	4694	ORS	GLU	ĸ	36	86.646	28.689	8.253	1.00 27.12	E
			GTA		36	91.413	26.630	6.826	1.00 23.40	E
MOTA	4695	C						5.645	1.00 23.72	E
MOTA	4696	0	GLU	E	36	91.252	26.347			
MOTA	4697	N	ILE	Е	37	91.576	25.707	7.767	1.00 23.97	E
MOTA	4698	CA	ILE	E	37	91.579	24.294	7.419	1.00 24.33	E
		CB	ILE		37	92.818	23.578	8.019	1.00 24.98	E
MOTA	4699							7.532	1.00 24.26	E
MOTA	4700		ILE		37	94.096	24.255			E
ATOM	4701	CG:	LILE	Е	37	92.771	23.616	9.544	1.00 25.10	
ATOM	4702	CD:	LILE	E	37	93.822	22.742	10.204	1.00 26.49	E
ATOM	4703	С	ILE		37	90.301	23.555	7.836	1.00 23.49	E
					37	89.871	22.627	7.162	1.00 23.62	В
MOTA	4704	0	IFR							E
MOTA	4705	N	VAL	E	38	89.690	23.975	8.936	1.00 25.16	
ATOM	4706	CA	VAL	E	38	88.465	23.342	9.415	1.00 25.85	B
ATOM	4707	CB	VAL		38	88.715	22.489	10.667	1.00 26.44	E
						87.516	21.610	10.932	1.00 27.10	E
MOTA	4708		1 VAL		38				1.00 29.59	E
MOTA	4709	CG:	2 VAL	В	38	89.980	21.671	10.495		
ATOM	4710	C	VAL	E	38	87.481	24.428	9.792	1.00 24.45	E
MOTA	4711	0	VAL	E	38	87.885	25.471	10.288	1.00 24.36	E
					39	86.193	24.168	9.594	1.00 24.90	E
MOTA	4712	N	ARG					9.904	1.00 23.66	E
ATOM	4713	CA	ARG	E	39	85.175	25.161			
MOTA	4714	CB	ARG	E	39	84.975	26.055	8.678	1.00 25.55	E
ATOM	4715		ARG	E	39	83.956	27.174	8.857	1.00 29.11	E
					39	83.514	27.755	7.515	1.00 29.37	B
MOTA	4716					84.626		6.739	1.00 29.70	E
ATOM	4717				39				1.00 31.37	E
MOTA	4718				39	84.505		5.516		
ATOM	4719	NH	1 ARG	E	39	83.314	28.842	4.930	1.00 33.54	E
ATOM	4720		2 ARG		39	85.572	29.266	4.879	1.00 27.78	E
						83.813		10.328		E
MOTA	4721		ARG		39					E
ATOM	4722	0	ARG	E		83.385		9.853		
ATOM	4723	N	PHE	E	40	83.147		11.242		E
MOTA	4724				40	81.799	24.918	11.655		E
						81.682			1.00 21.36	E
MOTA	4725									E
MOTA	4726					80.296				E
ATOM	4727	CI	1 PHE	E	40	79.944				
ATOM	4728		2 PHE			79.315	25.004	13.875		E
			1 PHE			78.628			1.00 17.84	B
ATOM	4729									E
MOTA	4730		2 PHE			78.001				E
MOTA	4731	L CZ	PHE	3 E	40	77.661	23.248	14.003	1.00 10.01	-

MOTA	4732	C	PHE	E	40	80.938	26.148	11.395	1.00 21.77	E
MOTA	4733	0		E	40	81.064	27.167	12.071 10.404	1.00 20.81 1.00 21.82	e
ATOM	4734	N	ASP		41 41	80.067 79.181	26.033 27.110	9.995	1.00 21.76	E
MOTA	4735 4736	CA CB	ASP ASP		41	79.101	27.182	8.470	1.00 22.62	B
MOTA MOTA	4737	CG		E	41	78.492	28.400	7.929	1.00 23.09	E
MOTA	4738			E	41	77.507	28.864	8.546	1.00 22.57	E
ATOM	4739		ASP	E	41	78.929	28.881	6.861	1.00 25.40	E
ATOM	4740	C	ASP	E	41	77.801	26.713	10.493	1.00 21.43	E
ATOM	4741	0	ASP		41	77.277	25.672	10.085	1.00 22.83	E
MOTA	4742	N	SER		42	77.210	27.520	11.369 11.895	1.00 19.04 1.00 20.39	E
ATOM	4743	CA	SER		42	75.896 75.399	27.173 28.220	12.907	1.00 19.13	E
ATOM	4744	CB OG	SER SER		42 42	75.271	29.505	12.323	1.00 24.30	B
ATOM ATOM	4745 4746	C	SER		42	74.891	27.000	10.762	1.00 20.23	E
ATOM	4747	ō	SER		42	73.916	26.267	10.910	1.00 18.97	B
ATOM	4748	N	ASP	E	43	75.145	27.660	9.631	1.00 21.77	B
ATOM	4749	CA	ASP		43	74.261	27.556	8.470	1.00 24.99	B
MOTA	4750	CB		E	43	74.561	28.651	7.439 7.727	1.00 26.10 1.00 28.71	E
ATOM	4751	CG	ASP		43	73.819 73.078	29.947 30.013	8.737	1.00 28.83	E
MOTA	4752 4753		ASP ASP		43 43	73.976	30.902	6.939	1.00 31.35	E
MOTA MOTA	4754	C	ASP		43	74.378	26.193	7.809	1.00 25.68	E
ATOM	4755	ō	ASP		43	73.424	25.727	7.190	1.00 28.27	E
ATOM	4756	N	VAL		44	75.544	25.558	7.937	1.00 25.47	E
MOTA	4757	CA	VAL	E	44	75.764	24.229	7.362	1.00 23.51	E
ATOM	4758	CB	VAL		44	77.251	24.007	6.964	1.00 24.39 1.00 19.52	E
MOTA	4759		VAL		44	77.456 77.655	22.579 24.984	6.491 5.867	1.00 13.32	E
ATOM	4760		VAL VAL		44 44	75.356	23.154	8.373	1.00 23.25	E
ATOM ATOM	4761 4762	0	VAL		44	74.774	22.136	8.005	1.00 22.01	E
ATOM	4763	N	GLY		45	75.683	23.370	9.644	1.00 22.52	E
ATOM	4764	CA	GLY		45	75.292	22.411	10.664	1.00 21.82	B
ATOM	4765	C	GLY	E	45	76.275	21.311	11.001	1.00 22.07	E
MOTA	4766	0	GLY		45	75.982	20.442	11.818	1.00 22.49	e
MOTA	4767	N	GLU		46	77.439	21.317	10.373 10.691	1.00 22.18 1.00 23.77	E
MOTA	4768	CA	GLU		46 46	78.421 78.147	20.295 19.017	9.891	1.00 26.29	E
MOTA	4769 4770	CB	GLU		46	78.455	19.112	8.411	1.00 28.23	E
ATOM ATOM	4771	CD	GLU		46	78.214	17.795	7.677	1.00 32.67	E
ATOM	4772	OE1			46	78.575	17.706	6.482	1.00 33.19	E
MOTA	4773	OE2	GLT	E	46	77.661	16.855	8.290	1.00 33.19	E
ATOM	4774	C	GLU		46	79.807	20.839	10.383	1.00 23.15	E
ATOM	4775	0	GLU		46	79.943	21.880 20.153	9.747 10.857	1.00 23.06 1.00 21.79	E
ATOM	4776	N	PHE		47 47	80.835 82.192	20.133	10.599	1.00 22.22	E
MOTA MOTA	4777 4778	CA CB	PHE		47	83.175	19.864	11.515	1.00 22.30	E
ATOM	4779	CG	PHE		47	83.058	20.249	12.968	1.00 22.20	E
ATOM	4780		L PHI		47	83.867	21.246	13.508	1.00 19.80	E
MOTA	4781		PHI		47	82.151	19.598	13.802	1.00 23.06	B
MOTA	4782		L PHI		47	83.781	21.585	14.858	1.00 18.93 1.00 22.63	E
MOTA	4783		2 PHI		47	82.055 82.872	19.931 20.925	15.157 15.684	1.00 20.81	E
MOTA	4784	CZ	PHI	SE	47 47	82.513	20.323	9.147	1.00 24.14	E
MOTA MOTA	4785 4786	0		EE		82.064	19.258		1.00 23.25	E
MOTA	4787	N		3 E		83.272			1.00 22.66	E
ATOM	4788		AR	3 E	48	83.672			1.00 23.86	B
ATOM	4789	CB		3 E		82.801			1.00 23.48 1.00 25.01	E E
MOTA	4790			G E		81.339			1.00 25.01	E
ATOM	4791			GE		81.155 79.747				E
ATOM	4792 4793			g e g e		79.038				E
MOTA MOTA	4794		1 AR			79.604				E
MOTA	4795		2 AR			77.763		3.946		B
ATOM	4796			G E	48	85.119				E
MOTA	4797			G E		85.507				E
MOTA	4798			AE		85.924				E
MOTA	4799			AE		87.316 88.102				E
MOTA	4800			A E		87.290				E
MOTA MOTA	4802			AI		86.507	_		1.00 23.16	E
ATOM	4803			L		88.108		5.050	1.00 23.56	E
ATOM	4804			T I		88.135	23.879			E
ATOM	480			L E		88.059	25.360	4.478	1.00 24.14	E

ATOM	4806	CG1	VAL	B	50	88.341	25.408	5.959	1.00 24.71	E
ATOM	4807	CG2	VAL	E	50	89.010	26.268	3.704	1.00 22.47	E
MOTA	4808	C	VAL	E	50	89.374	23.578	3.098	1.00 23.50	E
MOTA	4809	0	VAL		50	89.485	24.041	1.963	1.00 24.92	E
ATOM	4810	N	THR		51	90.281	22.770	3.650	1.00 24.49	E
ATOM	4811	CA	THR		51	91.492	22.317	2.951	1.00 25.50	E
MOTA	4812	CB	THR		51	92.742	23.198	3.234	1.00 25.69	E
ATOM	4813		THR		51	93.171	23.007	4.586	1.00 27.89	E
MOTA	4814	CG2			51	92.443	24.670	2.985	1.00 23.29 1.00 26.59	B
ATOM	4815	C	THR		51	91.817	20.895 20.477	3.420 4.496	1.00 20.35	B
ATOM	4816	0	THR		51	91.387 92.576	20.154	2.617	1.00 28.03	12
ATOM ATOM	4817 4818	N CA	LEU		52 52	92.949	18.783	2.956	1.00 28.49	E
ATOM	4819	CB	PEO		52		18.259	1.969	1.00 30.33	E
ATOM	4820	CG	LEU		52	93.536	17.892	0.556	1.00 34.17	E
ATOM	4821		LEU		52	94.749	17.628	-0.334	1.00 34.41	B
ATOM	4822		LEU		52	92.644	16.668	0.620	1.00 34.30	E
ATOM	4823	С	LEU		52	93.494	18.645	4.374	1.00 28.20	B
MOTA	4824	0	LEU	B	52	93.304	17.624	5.027	1.00 29.17	E
MOTA	4825	N	LEU	E	53	94.179	19.677	4.839	1.00 28.30	E
MOTA	4826	CA	LEU	B	53	94.766	19.682	6.171	1.00 28.75	B
MOTA	4827	CB	LEU	E	53	95.490	21.015	6.387	1.00 30.37	B
MOTA	4828	CG	LEU		53	96.939	21.010	6.882	1.00 32.74	E
MOTA	4829		LEU		53	97.777	20.085	6.008	1.00 31.60	E
MOTA	4830		LEU		53	97.498	22.444	6.854	1.00 30.06	E
MOTA	4831	C	LEU		53	93.727	19.464	7.278	1.00 27.82	E
MOTA	4832	0	LEU		53	94.027	18.858	8.312	1.00 25.47	E
ATOM	4833	N	GLY		54	92.508	19.957 19.813	7.059 8.062	1.00 27.39 1.00 26.92	E
ATOM	4834	CA	GLY		54	91.466 90.569	18.589	7.949	1.00 28.33	E
ATOM	4835	C	GLY		54 54	89.725	18.348	8.813	1.00 28.02	В
ATOM ATOM	4836 4837	O N	LEU		55	90.755	17.801	6.898	1.00 29.28	E
ATOM	4838	CA	PEO		55	89.930	16.620	6.675	1.00 31.43	E
ATOM	4839	СВ	LEU		55	90.410	15.885	5.419	1.00 32.39	E
ATOM	4840	CG	LEU		55	89.426	14.934	4.731	1.00 35.68	E
ATOM	4841		LEU		55	88.086	15.627	4.504	1.00 34.41	E
ATOM	4842		LEU		55	90.018	14.473	3.406	1.00 35.99	E
MOTA	4843	C	LEU	E	55	89.865	15.659	7.867	1.00 32.09	E
MOTA	4844	0	LEU	В	55	88.778	15.294	8.312	1.00 32.58	E
MOTA	4845	N	PRO	E	56	91.023	15.235	8.402	1.00 31.67	E
MOTA	4846	CD	PRO	E	56	92.411	15.520	8.000	1.00 31.37	E
MOTA	4847	CA	PRO		56	90.986	14.316	9.546	1.00 31.17	E
MOTA	4848	CB	PRO		56	92.459	14.163	9.919	1.00 30.50	e
MOTA	4849	CG	PRO		56	93.161	14.352	8.611 10.708	1.00 31.19 1.00 31.43	E
ATOM	4850	C	PRO PRO		56 56	90.158 89.250	14.865 14.195	11.205	1.00 32.17	E
MOTA	4851	O N	ALA		50 57	90.473	16.086	11.138	1.00 29.94	B
MOTA MOTA	4852 4853	CA	ALA		57	89.748	16.709	12.244	1.00 28.45	E
MOTA	4854	CB	ALA		57	90.314	18.098	12.532	1.00 27.09	B
ATOM	4855	C	ALA		57	88.249	16.807	11.960	1.00 27.57	E
ATOM	4856	o	ALA		57	87.436	16.466	12.812	1.00 26.57	B
ATOM	4857	N	ALA	E	58	87.899	17.270	10.761	1.00 27.40	E
ATOM	4858	CA	ALA	E	58	86.505	17.422	10.349	1.00 28.85	E
ATOM	4859	СВ	ALA	B	58	86.439	18.007	8.939	1.00 27.80	B
MOTA	4860	C	ALA		58	85.726	16.110	10,406	1.00 30.37	E
ATOM	4861	0	ALA		58	84.624	16.058	10.954	1.00 29.58	B
ATOM	4862	И	GLU		59	86.292	15.052	9.837	1.00 32.24	E
MOTA	4863	CA	GLU		59	85.632	13.750	9.845	1.00 35.22 1.00 36.81	E
MOTA	4864	СВ	GLU		59	86.441	12.724	9.049 7.549	1.00 40.89	. B
ATOM	4865	CG	GLU		59	86.392	12.917 11.775	6.805	1.00 44.28	E
ATOM	4866	CD	GLU L GLU		59 59	87.057 88.291		6.955	1.00 45.76	E
MOTA	4867		2 GPA		59	86.342		6.075	1.00 45.12	E
MOTA MOTA	4868 4869	C C	GLU GLU		59	85.441		11.260	1.00 34.08	B
MOTA	4870	o	GLU		59	84.384		11.596	1.00 34.48	E
MOTA	4871	N	TYR		60	86.466		12.090	1.00 33.21	E
ATOM	4872		TYR		60	86.390		13.463	1.00 32.36	E
ATOM	4873	СВ	TYR		60	87.724		14.177	1.00 33.78	B
ATOM	4874		TYR		60	87.657		15.594	1.00 35.68	E
MOTA	4875		1 TYR		60	87.543		15.872	1.00 37.48	E
MOTA	4876		1 TYR			87.394		17.173		E
MOTA	4877				60	87.628		16.655		E
MOTA	4878				60	87.478		17.965		E
MOTA	4879	CZ	TYP	E	60	87.360		18.218	1.00 41.88	E
							c	0		

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ATOM	4880	OH	TYR		60	87.198	11.262	19.508	1.00 44.51	E
ATOM	4881	C	TYR	E	60	85.312	13.623	14.275	1.00 32.30	E
ATOM	4882	0	TYR	E	60	84.430	12.976	14.839	1.00 30.56	E
MOTA	4883	N	TRP	E	61	85.391	14.950	14.347	1.00 31.42	E
ATOM	4884	CA	TRP	E	61	84.412	15.715	15.112	1.00 31.35	B
ATOM	4885	СВ	TRP		61.	84.744	17.219	15.071	1.00 32.78	E
		CG	TRP		61	86.051	17.584	15.748	1.00 35.14	E
ATOM	4886					86.909	18.687	15.425	1.00 37.07	B
ATOM	4887		TRP		61				1.00 37.15	E
ATOM	4888		TRP		61	87.994	18.655	16.331		
MOTA	4889	CE3	TRP	E	61	86.864	19.706	14.458	1.00 39.50	E
MOTA	4890	CD1	TRP	E	61	86.635	16.947	16.809	1.00 35.82	E
ATOM	4891	NEI	TRP	E	61	87.800	17.582	17.163	1.00 35.66	B
ATOM	4892		TRP		61	89.034	19.602	16.300	1.00 38.95	B
ATOM	4893		TRP		61	87.902	20.656	14.427	1.00 41.16	В
			TRP		61	88.971	20.591	15.346	1.00 40.81	R
ATOM	4894					82.968	15.472	14.653	1.00 29.29	E
MOTA	4895	C	TRP		61					E
ATOM	4896	0	TRP		61	82.045	15.563	15.458	1.00 29.20	
ATOM	4897	N	asn	E	62	82.772	15.162	13.373	1.00 27.86	E
ATOM	4898	CA	ASN	E	62	81.428	14.902	12.853	1.00 29.09	E
ATOM	4899	CB	ASN	E	62	81.379	15.051	11.331	1.00 29.42	E
ATOM	4900	CG	ASN	E	62	81.241	16.492	10.893	1.00 31.22	E
ATOM	4901		ASN		62	80.563	17.288	11.545	1.00 29.56	E
ATOM	4902		ASN		62	81.870	16.834	9.772	1.00 31.73	E
						80.906	13.519	13,220	1.00 28.26	E
MOTA	4903	C	ASN		62				1.00 27.48	E
MOTA	4904	0	ASN		62	79.716	13.242	13.086		
MOTA	4905	И	SER	B	63	81.795	12.647	13.672	1.00 27.47	E
MOTA	4906	CA	SER	E	63	81.381	11.311	14.056	1.00 29.39	E
ATOM	4907	CB	SER	E	63	82.511	10.310	13.803	1.00 28.56	E
ATOM	4908	OG	SER	E	63	83.607	10.545	14.671	1.00 32.72	E
MOTA	4909	C	SER		63	80.987	11.310	15.534	1.00 30.11	E
		ō	SER		63	80.515	10.297	16.055	1.00 31.52	E
ATOM	4910						12.453	16.196	1.00 28.86	E
ATOM	4911	N	GLN		64	81.173			1.00 28.28	E
MOTA	4912	CA	GLN		64	80.834	12.604	17.612		
ATOM	4913	CB	GLN	E	64	81.929	13.379	18.350	1.00 29.50	E
MOTA	4914	CG	GLN	E	64	83.330	12.787	18.266	1.00 29.72	E
MOTA	4915	æ	GLN	E	64	83.418	11.412	18.888	1.00 32.69	E
ATOM	4916	OE1	GLN	E	64	83.055	10.405	18.267	1.00 35.22	В
ATOM	4917	NE2			64	83.887	11.358	20.128	1.00 31.92	E
ATOM	4918	C	GLN		64	79.522	13.366	17.783	1.00 28.42	E
		ō	GLN		64	79.525	14.599	17.800	1.00 27.68	B
ATOM	4919						12.648	17.926	1.00 27.17	E
MOTA	4920	N	LYS		65	78.410				B
MOTA	4921	CA	LYS		65	77.111	13.300	18.097	1.00 29.82	
ATOM	4922	CB	LYS	E	65	75.994	12.258	18.253	1.00 31.43	B
MOTA	4923	CG	LYS	E	65	75.479	11.692	16.936	1.00 37.61	E
MOTA	4924	CD	LYS	E	65	74.801	12.766	16.072	1.00 41.12	E
ATOM	4925	CE	LYS	E	65	73.489	13.267	16.696	1.00 44.25	E
ATOM '	4926	NZ	LYS		65	72.832	14.322	15.861	1.00 44.10	E
	4927	c	LYS		65	77.067	14.273	19.278	1.00 28.07	E
ATOM						76.406	15.308	19.211	1.00 27.46	E
ATOM	4928	0	LYS		65				1.00 27.40	E
MOTA	4929	N	ASE		66	77.758	13.938	20.361		
MOTA	4930	CA	ASI		66	77.783	14.809	21.532	1.00 26.85	E
MOTA	4931	CB	ASI	E	66	78.566	14.142	22.670	1.00 26.10	E
ATOM	4932	CG	ASI) E	66	79.899	13.576	22.212	1.00 29.25	E
ATOM	4933	OD1	ASI	E	66	79.915	12.836	21.205	1.00 28.95	B
ATOM	4934	OD2	ASI) E	66	80.929	13.858	22.864	1.00 31.03	E
MOTA	4935	C	ASI		66	78.390	16.174	21.193	1.00 26.21	E
	4936	ō	ASI		66	77.844	17.215	21.559	1.00 26.58	E
MOTA						79.510	16.170	20.478	1.00 26.25	E
MOTA	4937	N	ILI		67				1.00 25.76	E
ATOM	4938	CA	IL		67	80.164	17.414	20.100		
MOTA	4939	CB	IL		67	81.551	17.153	19.477	1.00 27.31	E
ATOM	4940	CG2	IL	ΞE	67	82.261	18.467	19.210	1.00 25.90	E
MOTA	4941	CG1	IL	ΞE	67	82.396	16.304	20.429	1.00 28.85	B
MOTA	4942	CDI	IL	E E	67	82.494	16.871	21.844	1.00 32.35	E
ATOM	4943	C		E E	67	79.307		19.108	1.00 25.95	E
		Ö		e e	67	79.125			1.00 26.97	В
ATOM	4944					78.775			1.00 26.05	E
MOTA	. 4945	N		J E						E
MOTA	4946	CA		ÜΕ		77.927			1.00 26.36	
MOTA	4947	CB		UE		77.382			1.00 26.91	B
MOTA	4948	CG		UB		78.154			1.00 27.01	E
MOTA	4949	CD:	LLE	UB	68	77.389	16.002	13.913	1.00 26.26	E
MOTA	4950	CD	LE	V E	68	78.311	18.342	14.076	1.00 24.04	E
ATOM	4951	c		U E		76.760			1.00 26.03	E
MOTA	4952	ō		UE		76.433				E
		Ŋ		UE		76.134				E
MOTA	4953	44	ىد							_

75.000 18.726 19.471 1.00 30.38 ATOM 4954 CA GLU E 69 74.481 17.720 CB GLU E 69 20.508 1.00 34.06 ATOM 4955 19.989 ATOM 4956 CG GLU E 69 73.426 16.742 1.00 40.55 1.00 44.43 MOTA 4957 CD GLU E 69 72.211 17.444 19.392 MOTA 4958 OB1 GLU E 69 71.802 18.505 19.922 1.00 43.73 OB2 GLU E 69 71.656 16.926 18.397 1.00 48.15 ATOM 4959 ATOM 4960 C GLU E 69 75.335 20.034 20.178 1.00 29.17 4961 GLU E 69 74.587 21.009 20.071 1.00 29.71 ATOM 0 ATOM 4962 N ARG E 70 76.453 20.059 20.899 1.00 26.65 CA ARG E 70 76.844 21.262 ATOM 21.620 1.00 25.51 4963 MOTA 4964 CB ARG E 70 78.001 20.965 22.572 1.00 27.14 MOTA 4965 CG ARG E 70 77.711 19.855 23.563 1.00 31.22 MOTA CD ARG E 70 78.637 19.934 24.769 1.00 35.11 4966 78.758 18.647 ATOM 4967 NE ARG E 70 25,440 1.00 39,19 R 4968 CZ ARG E 70 79.456 17.628 24.956 1.00 41.08 MOTA B 80.096 17.752 ATOM NH1 ARG E 70 23.802 1.00 45.32 4969 NH2 ARG E 70 ATOM 4970 79.511 16.486 25.618 1.00 44.01 E ARG E 70 MOTA 4971 C 77.230 22.395 20.677 1.00 24.57 R ARG B 70 76.927 23.557 20.941 1.00 21.44 ATOM 4972 0 LYS E 71 77.897 22.057 19.576 1.00 24.56 ATOM 4973 N LYS E 71 CA 78.309 23.071 18.612 1.00 24.08 ATOM 4974 MOTA 4975 CB LYS E 71 79.202 22.452 17.534 1.00 25.39 LYS E 71 80.100 23.474 16.852 1.00 29.73 ATOM 4976 CG MOTA 4977 CD LYS E 71 81.067 24.095 17.862 1.00 30.94 CE LYS E 71 NZ LYS E 71 81.905 25.205 17,256 1.00 31.82 R ATOM 4978 18.290 1.00 33.45 ATOM 4979 82.774 25.849 LYS E 71 77.087 23.732 17.960 1.00 22.42 MOTA 4980 C MOTA 4981 0 LYS E 71 77.045 24.951 17.780 1.00 18.65 ARG E 72 76.092 22.919 17.620 1.00 22.31 ATOM 4982 N 74.867 23.419 17.002 1.00 21.44 ATOM 4983 CA ARG E 72 E MOTA 4984 CB ARG E 72 73.984 22.250 16.578 1.00 19.93 E CG ARG E 72 74.534 21.497 15.407 1.00 21.45 ATOM 4985 ARG E 72 73.779 20.223 15.141 1.00 23.34 Е MOTA 4986 CD 74.211 19.643 NE ARG E 72 13.877 1.00 24.99 MOTA 4987 Е ATOM 4988 CZ ARG E 72 74.028 18.377 13.522 1.00 27.42 \mathbf{E} 14.344 1.00 25.90 MOTA 4989 NH1 ARG E 72 73.411 17.533 NH2 ARG B 72 12.341 1.00 25.41 74,475 17.955 4990 ATOM 17.961 1.00 21.34 ATOM 4991 C ARG E 72 74.093 24.315 E 4992 ARG E 72 73.336 25.182 17.535 1.00 23.67 R ATOM 0 N ALA E 73 74.293 24.105 19.256 1.00 21.13 MOTA 4993 CA ALA E 73 73.610 24.887 20.281 1.00 22.11 ATOM 4994 CB ALA E 73 ATOM 4995 73.476 24.052 21.568 1.00 21.20 4996 ALA E 73 74.347 26.189 20.576 1.00 22.67 ATOM С ATOM 4997 0 ALA B 73 73.773 27.133 21.125 1.00 25.58 Е ALA E 74 75.614 26.248 20.195 1.00 22.52 ATOM 4998 N CA ALA E 74 76.420 27.432 20.448 1.00 22.20 ATOM 4999 5000 CB ALA E 74 77.830 27.219 19.910 1.00 24.81 ATOM 19.882 1.00 22.28 ATOM 5001 ALA E 74 75.828 28.722 C ALA E 74 76.027 29.796 20.452 1.00 20.24 E ATOM 5002 0 VAL E 75 18,770 1,00 21.92 MOTA 5003 N 75.102 28.634 Е ATOM 5004 CA VAL E 75 74.519 29.841 18.185 1.00 21.69 ATOM 5005 CB VAL E 75 73.700 29.517 16.890 1.00 22.61 CG1 VAL E 72.488 28,657 17.219 1.00 24.39 5006 75 Е ATOM 16.218 1.00 24.00 MOTA 5007 CG2 VAL E 75 73.270 30.798 E 5008 VAL E 75 73.639 30.558 19.219 1.00 21.26 E ATOM C MOTA 5009 0 VAL E 75 73.464 31.777 19.164 1.00 20.64 ASP E 73.106 29.802 20.171 1.00 20.84 В 5010 N 76 ATOM 30.385 21.220 1.00 23.98 ATOM 5011 CA ASP E 76 72.273 Е ATOM 5012 CB ASP E 76 71.022 29.532 21.471 1.00 25.33 E 70.010 20.331 1.00 27.46 MOTA 5013 CG ASP E 76 29.605 E OD1 ASP B 69.807 30.697 19.763 1.00 29.45 5014 76 MOTA OD2 ASP E 76 69.398 28.566 20.020 1.00 31.17 ATOM 5015 MOTA 5016 С ASP E 76 73.044 30.525 22.538 1.00 24.46 R 72.910 31.524 23.247 1.00 25.64 MOTA 5017 0 ASP E 76 ARG E 73.846 29.515 22.855 1.00 23.56 MOTA 5018 N 77 29.486 74.627 24.085 1.00 22.99 MOTA 5019 CA ARG E 77 MOTA 5020 CB ARG E 77 75.176 28.077 24.279 1.00 26.55 ARG E 77 75.848 27.806 25.607 1.00 33.45 MOTA 5021 CG 25.825 1.00 37.66 CD ARG E 77 ATOM 5022 75.961 26.295 NE ARGE 77 25.883 1.00 40.99 ATOM 5023 74.639 25.666 CZ ARG E 77 74.423 24.352 25.862 1.00 43.13 MOTA 5024 ATOM 5025 NH1 ARG E 77 75.438 23.503 25.782 1.00 43.11 NH2 ARG E 77 25.914 1.00 44.93 MOTA 5026 73.183 23.885 75.763 30.509 24.078 1.00 23.23 C ARG E 77 MOTA 5027

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MOTA	5028	0	ARG			76.162	31.022	25.129	1.00 23.14	B
ATOM	5029	N	VAL			76.275	30.808	22.889	1.00 20.54	B
ATOM ATOM	5030 5031	CA CB	VAL		78	77.354	31.767	22.741	1.00 19.56	E
ATOM	5031		VAL VAL		78 78	78.500	31.181	21.891	1.00 19.17	E
ATOM	5033		VAL		78	79.612 79.032	32.208 29.921	21.724 22.541	1.00 17.69	E
ATOM	5034	C	VAL		78	76.888	33.075	22.093	1.00 19.40	E
ATOM	5035	0	VAL		78	76.786	34.110	22.756	1.00 21.57	E
ATOM	5036	N	CYS	E	79	76.595	33.021	20.799	1.00 17.88	E
ATOM	5037	CA	CYS	E	79	76.181	34.205	20.059	1.00 17.48	E
ATOM	5038	C	CYS		79	74.967	34.966	20.620	1.00 18.40	В
ATOM	5039	0	CYS		79	75.087	36.146	20.967	1.00 16.69	E
MOTA MOTA	5040 5041	CB SG	CYS		79	75.946	33.847	18.592	1.00 17.30	E
ATOM	5041	N	CYS		79 80	77.361 73.802	33.071	17.722	1.00 27.04	E
MOTA	5043	CA	ARG		80	72.641	34.326 35.050	20.717 21.240	1.00 17.59 1.00 20.01	E
ATOM	5044	CB	ARG		80	71.340	34.256	21.032	1.00 20.22	e
ATOM	5045	CG	ARG	E	80	70.886	34.213	19.584	1.00 22.92	E
ATOM	5046	CD	ARG		80	69.423	33.811	19.439	1.00 23.91	E
ATOM	5047	NB	ARG		80	68.972	33.965	18.057	1.00 23.49	E
ATOM	5048	CZ	ARG		80	69.206	33.089	17.082	1.00 25.16	E
ATOM	5049		ARG		80	69.884	31.975	17.326	1.00 24.15	E
ATOM ATOM	5050 5051	NH2	ARG		80 80	68.778	33.336	15.851	1.00 25.51	E
ATOM	5051	0	ARG		80	72.804 72.317	35.423 36.464	22.716	1.00 20.35	E
ATOM	5053	N	HIS		81	73.495	34.581	23.153 23.479	1.00 17.98 1.00 21.22	E
ATOM	5054	CA	HIS		81	73.717	34.867	24.895	1.00 21.22	E
MOTA	5055	CB	HIS		81	74.467	33.717	25.572	1.00 24.38	E
ATOM	5056	CG	HIS	B	81	74.955	34.046	26.950	1.00 26.42	E
ATOM	5057		HIS		81	76.188	34.381	27.404	1.00 26.61	E
ATOM	5058		HIS		81	74.122	34.080	28.048	1.00 26.60	E
ATOM ATOM	5059		HIS		81	74.819	34.420	29.117	1.00 25.75	E
MOTA	5060 5061	C	HIS HIS		81 81	76.075 74.531	34.609	28.754	1.00 26.16	E
ATOM	5062	ō	HIS		81	74.531	36.146 37.076	25.060 25.742	1.00 21.41 1.00 19.84	e
ATOM	5063	N	ASN		82	75.700	36.188	24.426	1.00 22.13	E
MOTA	5064	CA	ASN	E	82	76.568	37.361	24.535	1.00 21.51	E
ATOM	5065	CB	asn		82	77.927	37.111	23.864	1.00 18.47	B
ATOM	5066	CG	asn		82	78.702	35.982	24.515	1.00 18.09	E
ATOM	5067		ASN		82	78.453	35.632	25.669	1.00 19.05	E
ATOM ATOM	5068 ·	C WDS	ASN ASN		82	79.656	35.409	23.777	1.00 15.06	E
ATOM	5070	Ö	ASN		82 82	75.936 76.212	38.612 39.716	23.949	1.00 20.33	E
ATOM	5071	N	TYR		83	75.089	38.454	24.412 22.940	1.00 22.84 1.00 19.71	e
ATOM	5072	CA	TYR		83	74.454	39.620	22.336	1.00 20.96	B
ATOM	5073	CB	TYR	E	83	73.619	39.211	21.114	1.00 21.58	В
ATOM	5074	CG	TYR		83	73.223	40.368	20.218	1.00 22.56	B
ATOM	5075		TYR		83	72.047	41.090	20.439	1.00 23.70	E
ATOM	5076		TYR		83	71.682	42.152	19.593	1.00 25.46	E
ATOM ATOM	5077 5078		TYR TYR		83	74.027	40.736	19.140	1.00 22.35	B
ATOM	5079	CZ	TYR		83 83	73.675 72.508	41.788 42.491	18.297 18.523	1.00 24.48	E
ATOM	5080	ОН	TYR		83	72.185	43.524	17.671	1.00 26.06 1.00 28.63	E
ATOM	5081	С	TYR		83	73.583	40.345	23.363	1.00 21.22	E
ATOM	5082	0	TYR	E	83	73.399	41.557	23.276	1.00 21.25	E
ATOM	5083	N	GLN		84	73.046	39.606	24.333	1.00 22.94	E
MOTA	5084	CA	GLN		84	72.234	40.226	25.377	1.00 25.07	E
ATOM ATOM	5085	CB	GLN		84	71.631	39.180	26.324	1.00 25.76	B
ATOM	5086 5087	CD	GLN GLN		84	70.863	38.047	25.653	1.00 30.97	E
ATOM	5088		GLN		84 84	69.889 69.055	38.525 39.401	24.594 24.840	1.00 33.95	E
ATOM	5089		GLN		84	69.986	37.940	23.401	1.00 36.35 1.00 36.25	e
ATOM	5090	C	GLN		84	73.158	41.145	26.174	1.00 35.23	E
ATOM	5091	0	GLN		84	72.804	42.290	26.473	1.00 27.11	E
ATOM	5092	N	LEU		85	74.344	40.637	26.510	1.00 24.17	B
MOTA	5093	CA	LEU		85	75.330	41.413	27.256	1.00 26.47	E
ATOM	5094	CB	LEU		85	76.601	40.590	27.515	1.00 26.91	E
ATOM ATOM	5095 5096	CG	LEU		85 05	76.485	39.202	28.161	1.00 29.65	E
ATOM	5097		LEU		85 85	77.872 75.564	38.735 39.247	28.587 29.365	1.00 31.29	e
ATOM	5098	C	LEU		85	75.698	42.661	26.459	1.00 32.27 1.00 26.89	E
ATOM	5099	o	LEU		85	75.762	43.757	27.004	1.00 28.24	E
ATOM	5100	N	GLU		86	75.941	42.484	25.162	1.00 27.39	E
ATOM	5101	CA	GLU	E	86	76.293	43.603	24.295	1.00 28.02	E

MOTA	5102	СВ	GLU	E	86	76.492	43.126	22.852	1.00 26.60	E
ATOM	5103	CG	GLU		86	77.524	42.026	22.672	1.00 30.65	E
ATOM	5104	CD	GLU	E	86	78.942	42.457	23.024	1.00 31.17	E
MOTA	5105		GLU		86	79.860	41.612	22.919	1.00 31.68	В
MOTA	5106		GLU		86	79.139	43.631	23.402	1.00 31.77	E
ATOM	5107	C	GLU		86	75.165	44.630	24.327	1.00 27.95	E
MOTA	5108	0	GLU		86	75.407	45.834	24.257	1.00 24.30 1.00 28.96	E
ATOM	5109	N CA	LEU		87 87	73.935 72.736	44.130 44.962	24.442 24.468	1.00 28.96	E
MOTA MOTA	5110 5111	CB	PEA		87	71.496	44.062	24.423	1.00 32.64	E
ATOM	5112	CG	LEU		87	70.506	44.100	23.248	1.00 35.59	E
ATOM	5113		LEU		87	71.101	44.734	21.997	1.00 35.24	E
ATOM	5114		LEU		87	70.071	42.675	22.965	1.00 34.35	E
ATOM	5115	С	LEU	B	87	72.669	45.893	25.686	1.00 33.33	B
MOTA	5116	0	LEU	E	87	71.967	46.902	25.663	1.00 32.52	E
MOTA	5117	N	ARG		88	73.401	45.560	26.745	1.00 35.06	E
MOTA	5118	CA	ARG		88	73.399	46.389	27.948	1.00 37.29	E
MOTA	5119	CB	ARG		88	73.348	45.524	29.215	1.00 39.69	E
ATOM	5120	CG	ARG		88	72.471	44.275	29.158	1.00 43.37	e
ATOM	5121	CD	ARG		88	72.441 71.846	43.592 42.257	30.529 30.499	1.00 45.38 1.00 48.76	E
MOTA MOTA	5122 5123	NE CZ	ARG		88 88	70.625	41.985	30.047	1.00 50.95	B
ATOM	5124		ARG		88	69.854	42.958	29.579	1.00 52.23	E
ATOM	5125		ARG		88	70.171	40.738	30.064	1.00 51.26	E
ATOM	5126	C	ARG		88	74.670	47.225	28.010	1.00 37.36	E
ATOM	5127	0	ARG	E	88	74.842	48.044	28.913	1.00 37.55	B
MOTA	5128	N	THR	B	89	75.564	47.019	27.049	1.00 36.40	R
ATOM	5129	CA	THR		89	76.834	47.731	27.055	1.00 34.93	E
MOTA	5130	CB	THR		89	77.951	46.807	27.590	1.00 36.26	B
MOTA	5131	OG1			89	77.973	45.590	26.825	1.00 34.21	E
ATOM	5132	CG2	THR		89	77.708	46.478	29.056	1.00 33.95 1.00 33.37	e
MOTA	5133	C	THR		89 89	77.294 76.958	48.304 49.431	25.718 25.356	1.00 33.37	E
ATOM ATOM	5134 5135	O N	THR		90	78.080	47.510	25.000	1.00 32.11	E
ATOM	5136	CA	THR		90	78.639	47.895	23.712	1.00 30.45	E
ATOM	5137	СВ	THR		90	79.313	46.681	23.041	1.00 31.20	E
ATOM	5138		THR		90	80.238	46.086	23.958	1.00 32.67	E
ATOM	5139	CG2	THR	E	90	80.076	47.109	21.811	1.00 32.64	E
MOTA	5140	C	THR	E	90	77.639	48.504	22.738	1.00 28.40	E
MOTA	5141	0	THR		90	77.903	49.538	22.133	1.00 27.20	E
MOTA	5142	N	TEA		91	76.489	47.864	22.582	1.00 29.83	E
ATOM	5143	CA	PEA		91	75.482	48.361	21.655	1.00 29.52	E
MOTA	5144	CB	LEU		91	74.474	47.252 46.101	21.354 20.550	1.00 27.50 1.00 26.15	E
MOTA	5145 5146	CG	TEA TEA		91 91	75.091 74.102	44.959	20.350	1.00 24.51	B
ATOM ATOM	5147	CD2			91	75.487	46.593	19.157	1.00 23.04	E
ATOM	5148	C	LEU		91	74.770	49.629	22.129	1.00 30.74	E
MOTA	5149	ō	LEU		91	73.994	50.228	21.382	1.00 31.46	E
ATOM	5150	N	GLN		92	75.035	50.043	23.366	1.00 29.33	E
ATOM	5151	CA	GLN	E	92	74.427	51.259	23.884	1.00 30.04	E
MOTA	5152	CB	GLN	E	92	73.869	51.044	25.294	1.00 31.55	E
MOTA	5153	CG	GLN		92	72.500	50.381	25.327	1.00 36.90	E
MOTA	5154	CD	GLN		92	71.865	50.426	26.706	1.00 41.59	E
ATOM	5155		GLN		92	70.760 72.563	49.920 51.037	26.911 27.662	1.00 43.76 1.00 43.75	e
MOTA MOTA	5156 5157	NE2 C	GLN GLN		92 92	75.430	52.409	23.898	1.00 28.45	E
ATOM	5158	ō	GLN		92	75.059	53.558	24.125	1.00 28.57	B
ATOM	5159	N	ARG		93	76.699	52.098	23.650	1.00 26.37	E
ATOM	5160	CA	ARG		93	77.737	53.127	23.633	1.00 26.74	B
ATOM	5161	CB	ARG		93	79.112	52.513	23.340	1.00 24.84	E
ATOM	5162	CG	ARG	E	93	80.260	53.525	23.217	1.00 20.15	E
MOTA	5163	CD	ARG	E	93	81.569	52.801	22.894	1.00 20.06	E
MOTA	5164	NE	ARG		93	82.718	53.685	22.729	1.00 15.27	E
MOTA	5165	CZ	ARG		93	83.316	54.330	23.729	1.00 16.93	E
MOTA	5166		ARG		93	82.875	54.197	24.973	1.00 17.82 1.00 16.28	E
MOTA	5167		ARG		93	84.367	55.101 54.173	23.492 22.576	1.00 16.28	E
ATOM ATOM	5168 5169	0	ARG ARG		93 93	77.428 77.202	53.847	21.407	1.00 28.26	E
ATOM	5170	И	ARG		93 94	77.411	55.431	22.995	1.00 28.24	B
MOTA	5171	CA	ARG		94	77.159	56.529	22.084	1.00 29.74	E
ATOM	5172	СВ	ARG		94	75.661	56.855	22.053	1.00 32.88	E
ATOM	5173	CG	ARG		94	74.912	55.941	21.086	1.00 36.76	E
MOTA	5174	CD	ARG		94	73.402	56.055	21.163	1.00 40.38	E
MOTA	5175	NE	ARG	E	94	72.758	55.304	20.080	1.00 44.16	E

ATOM	5176	CZ	ARG	B	94	72.871	53.991	19.894	1.00 43.57	K
ATOM	5177	NH1	ARG	E	94	73.602	53.259	20.720	1.00 45.04	E
ATOM	5178		ARG		94	72.262	53.408	18.869	1.00 45.75	B
ATOM	5179	C	ARG		94	77.992	57.734	22.497	1.00 29.26	E
										E
MOTA	5180	0	ARG		94	77.773	58.331	23.546	1.00 30.32	
MOTA	5181	N	VAL		95	78.974	58.063	21.667	1.00 26.76	E
ATOM	5182	CA	VAL		95	79.859	59.188	21.936	1.00 25.75	E
MOTA	5183	CB	VAL	E	95	81.340	58.763	21.855	1.00 22.33	E
ATOM	5184	CG1	VAL	E	95	82.244	59.914	22.287	1.00 19.80	E
ATOM	5185	CG2	VAL	E	95	81.565	57.534	22.717	1.00 19.11	E
ATOM	5186	c	VAL		95	79.600	60.266	20.902	1.00 26.51	E
ATOM	5187	0	VAL		95	79.787	60.042	19.703	1.00 27.04	E
ATOM	5188	N	GLU		96	79.160	61.430	21.366	1.00 27.28	E
MOTA	5189	CA	GLU	B	96	78.870	62.536	20.466	1.00 28.16	E
MOTA	5190	CB	GĿΰ	B	96	78.260	63.716	21.227	1.00 30.40	E
MOTA	5191	CG	GLU	B	96	76.965	63.396	21.952	1.00 34.36	E
ATOM	5192	CD	GLU	В	96	76.348	64.625	22.609	1.00 36.84	E
ATOM	5193		GLU		96	75.295	64.478	23.272	1.00 38.81	B
ATOM	5194	OE2	GLU		96	76.914	65.734	22.460	1.00 35.73	B
MOTA	5195	C	Grū		96	80.148	62.987	19.793	1.00 25.65	B
MOTA	5196	0	GLU		96	81.176	63.171	20.440	1.00 24.93	Е
MOTA	5197	N	PRO	K	97	80.101	63.168	18.473	1.00 25.41	E
MOTA	5198	CD	PRO	E	97	78.977	62.979	17.539	1.00 24.36	B
ATOM	5199	CA	PRO	В	97	81.304	63.603	17.770	1.00 24.81	E
MOTA	5200	CB	PRO	Е	97	80.927	63.416	16.306	1.00 24.85	E
ATOM	5201	CG	PRO		97	79.456	63.717	16.309	1.00 25.36	E
ATOM	5202	c	PRO		97	81.643	65.048	18.089	1.00 24.48	E
										E
ATOM	5203	0	PRO		97	80.761	65.844	18.419	1.00 23.85	
ATOM	5204	N	THR		98	82.927	65.377	18.025	1.00 22.82	E
MOTA	5205	CA	THR		98	83.340	66.748	18.244	1.00 24.12	E
MOTA	5206	CB	THR	Е	98	84.679	66.852	19.019	1.00 26.31	E
MOTA	5207	OG1	THR	E	98	85.744	66.355	18.205	1.00 34.47	E
MOTA	5208	CG2	THR	E	98	84.623	66.049	20.302	1.00 23.83	B
MOTA	5209	C	THR		98	83.519	67.254	16.817	1.00 22.12	B
MOTA	5210	ŏ	THR		98	84.162	66.601	15.993	1.00 21.35	E
			VAL		99	82.923	6B.400	16.516	1.00 21.99	E
MOTA	5211	N								E
MOTA	5212	CA	VAL		99	83.001	68.957	15.177	1.00 20.67	
MOTA	5213	CB	VAL		99	81.585	69.217	14.619	1.00 19.57	E
MOTA	5214		VAL		99	81.667	69.645	13.154	1.00 14.62	E
ATOM	5215	CG2	VAL	E	99	80.732	67.944	14.766	1.00 15.20	E
MOTA	5216	C	VAL	K	99	83.814	70.240	15.158	1.00 22.05	E
MOTA	5217	0	VAL	E	99	83.524	71.194	15.884	1.00 22.27	E
MOTA	5218	N	THR	R	100	84.827	70.250	14.304	1.00 21.34	E
ATOM	5219	CA			100	85.728	71.376	14.176	1.00 23.10	E
							71.024	14.786	1.00 24.55	E
MOTA	5220	CB	THR			87.104				
MOTA	5221		THR			86.941	70.728	16.180	1.00 30.47	E
MOTA	5222		THR			88.079	72.183	14.634	1.00 27.79	E
MOTA	5223	С	THR	E	100	85.934	71.777	12.722	1.00 23.36	E
MOTA	5224	0	THR	E	100	86.024	70.926	11.842	1.00 21.77	E
MOTA	5225	N	ILE	В	101	86.009	73.082	12.473	1.00 24.40	E
ATOM	5226	CA	ILE	E	101	86.236	73.584	11.124	1.00 25.31	E
ATOM	5227	CB			101	85.092	74.518	10.645	1.00 24.21	E
ATOM	5228		ILE	_		85.398	75.044	9.245	1.00 22.51	E
	5229		ILE			83.760	73.768	10.636	1.00 24.86	E
ATOM										E
MOTA	5230		IFE			82.584	74.635	10.197	1.00 25.22	
MOTA	5231	C			101	87.538	74.372	11.116	1.00 26.66	B
MOTA	5232	0	ILE	B	101	87.859	75.065	12.074	1.00 26.18	B
ATOM	5233	N	SER	В	102	88.287	74.262	10.029	1.00 31.17	R
MOTA	5234	CA	SER	E	102	89.547	74.977	9.902	1.00 35.36	B
MOTA	5235	CB	SER	Е	102	90.619	74.306	10.755	1.00 34.20	E
ATOM	5236	OG			102	90.777	72.953	10.374	1.00 40.09	E
ATOM	5237	C			102	89.976	74.979	8.448	1.00 36.82	E
										В
MOTA	5238	0			102	89.913	73.953	7.777	1.00 36.68	
MOTA	5239	N			103	90.404	76.139	7.932	1.00 39.96	E
MOTA	5240	æ			103	90.458	77.473	8.553	1.00 40.07	E
ATOM	5241	CA	PRO	E	103	90.831	76.190	6.532	1.00 42.01	E
ATOM	5242	CB	PRO	E	103	90.856	77.682	6.237	1.00 41.76	E
MOTA	5243	CG	PRO	E	103	91.282	78.258	7.556	1.00 42.86	E
ATOM	5244	C			103	92.196	75.534	6.390	1.00 44.62	E
MOTA	5245	ō			103	92.943	75.430	7.365	1.00 44.53	E
ATOM	5246	И			104	92.514	75.086	5.181	1.00 47.92	E
ATOM						93.789	74.426	4.920	1.00 50.83	E
	5247	CA			104					E
MOTA	5248	CB			104	93.712	73.637	3.612	1.00 52.33	
MOTA	5249	OG	SER	E	104	94.904	72.901	3.396	1.00 55.60	E

3.0004		_							
ATOM	5250	С	SER	B 104	94.941	75.422	4.845	1.00 52.18	B
ATOM	5251	0	SER	E 104	96.080	75.093	5.186	1.00 53.53	E
ATOM	5252	N	ASN	E 113	90.669	78.112	-1.692	1.00 48.40	B
ATOM	5253	CA		E 113					
					90.651	77.795	-0.269	1.00 47.57	E
ATOM	5254	CB		E 113	89.863	78.854	0.496	1.00 51.34	E
ATOM	5255	CG	ASN :	Ē 113	90.504	80.219	0.417	1.00 52,99	E
ATOM	5256	OD1	ASN :	E 113	90.693	80.765	-0.670	1.00 55.11	E
ATOM	5257		ASN		90.845				
						80.781	1.572	1.00 55.09	E
ATOM	5258	C		E 113	90.045	76.424	-0.001	1.00 44.87	B
ATOM	5259	0	ASN :	B 113	89.374	75.852	-0.860	1.00 44.99	E
ATOM	5260	N	LEU :	E 114	90.282	75.904	1.197	1.00 41.65	B
ATOM	5261	CA		B 114	89.765				
						74.592	1.568	1.00 38.53	E
ATOM	5262	CB		B 114	90.823	73.521	1.287	1.00 38.84	B
MOTA	5263	CG	LEU 1	E 114	90.383	72.060	1.441	1.00 40.32	· B
MOTA	5264	CD1	LEU I	E 114	89.314	71.726	0.400	1.00 39.94	E
ATOM	5265		LEU I		91.586	71.145	1.266		
								1.00 40.52	E
ATOM	5266	C		E 114	89.349	74.523	3.036	1.00 34.78	E
ATOM	5267	0	TEO 1	E 114	90.173	74.684	3.929	1.00 33.51	E
ATOM	5268	N	LEU :	B 115	88.063	74.293	3.278	1.00 32.05	E
ATOM	5269	CA		E 115	87.550	74.181	4.641		
								1.00 29.68	E
ATOM	5270	CB		3 115	86.158	74.809	4.754	1.00 29.84	E
MOTA	5271	CG	LEU :	3 115	86.046	76.257	5.241	1.00 31.52	E
MOTA	5272	CD1	LEU I	3 115	87.101	77.140	4.574	1.00 32.51	E
ATOM	5273	CD2	LEU I	2 115	84.636	76.762	4.948	1.00 30.75	E
ATOM				3 115					
	5274	C			87.472	72.712	5.034	1.00 27.57	E
ATOM	5275	0		3 115	86.871	71.900	4.331	1.00 25.33	E
ATOM	5276	N	VAL 1	E 116	88.089	72.381	6.161	1.00 26.32	E
ATOM	5277	CA	VAL 1	3 116	88.099	71.014	6.651	1.00 24.42	В
ATOM	5278	CB	VAL 1		89.513	70.572	7.075	1.00 24.51	E
ATOM	5279		VAL 1						
					89.467	69.160	7.641	1.00 22.66	E
ATOM	5280		VAL 1		90.458	70.643	5.879	1.00 26.70	E
MOTA	5281	C	VAL 1	3 116	87.195	70.842	7.846	1.00 22.77	E
ATOM	5282	0	VAL 1	3 116	87.376	71.496	8.868	1.00 23.04	E
ATOM	5283	N	CYS 1	E 117	86.208	69.968	7.717	1.00 22.34	B
ATOM	5284	CA	CYS I		85.326	69.711	8.840	1.00 21.65	
ATOM	5285		CYS 1						E
		C			85.769	68.391	9.466	1.00 19.44	E
ATOM	5286	0	CYS 1		85.607	67.319	8.877	1.00 18.95	E
MOTA	5287	CB	CYS 1	3 117	83.863	69.626	8.401	1.00 22.57	E
MOTA	5288	SG	CYS I	3 117	82.771	69.420	9.844	1.00 25.79	E
ATOM	5289	N	SER I	118	86.355	68.488	10.654	1.00 19.92	E
ATOM	5290	CA	SER I		86.837	67.330			
							11.387	1.00 17.98	E
ATOM	5291	CB	SER I		88.115	67.671	12.146	1.00 18.33	E
ATOM	5292	OG	SER E		89.121	68.117	11.260	1.00 24.58	E
MOTA	5293	С	SER I	3 118	85.798	66.860	12.377	1.00 17.01	E
MOTA	5294	0	SER E	118	85.507	67.543	13.354	1.00 16.69	E
ATOM	5295	N	VAL E	119	85.240	65.688	12.112	1.00 16.58	E
ATOM	5296	CA	VAL I		84.242				
						65.095	12.985	1.00 16.03	B
MOTA	5297	CB	VAL E		83.040	64.582	12.160	1.00 15.47	E
MOTA	5298		VAL I		81.918	64.147	13.077	1.00 13.75	B
ATOM	5299	CG2	VAL E	119	82.559	65.686	11.216	1.00 10.95	B
ATOM	5300	C	VAL E	119	85.018	63.960	13.638	1.00 17.51	E
ATOM	5301	0	VAL E		85.238	62.906			
									E
MOTA	5302	N	THR E		85.442	64.203	14.871	1.00 18.44	E
MOTA	5303	CA	THR E		86.265	63.266	15.616	1.00 18.41	E
MOTA	5304	CB	THR E	120	87.562	63.962	16.042	1.00 18.11	E
MOTA	5305	OG1	THR E	120	87.242	65.078	16.887	1.00 17.18	B
MOTA	5306		THR E		88.304	64.481	14.835	1.00 16.77	E
ATOM	5307	c	THR E		85.655				
ATOM						62.656	16.875	1.00 20.11	E
	5308	0	THR E		84.665	63.148	17.417	1.00 21.96	. B
ATOM	5309	N	ASP E	3 121	86.272	61.566	17.319	1.00 19.96	E
ATOM	5310	CA	ASP E	121	85.882	60.864	18.529	1.00 21.06	E
ATOM	5311	CB	ASP E	121	86.313	61.686	19.745	1.00 25.93	E
ATOM	5312	CG	ASP E		87.814	61.765	19.882	1.00 30.02	E
ATOM	5313		ASP E		88.291	62.524			
							20.756	1.00 34.97	E
ATOM	5314		ASP E		88.513	61.063	19.114	1.00 31.15	E
MOTA	5315	C	ASP E		84.431	60.463	18.709	1.00 20.39	B
MOTA	5316	0	ASP E	121	83.857	60.698	19.766	1.00 22.05	B
ATOM	5317	N	PHE F	122	83.827	59.841	17.708	1.00 19.69	E
MOTA	5318	CA	PHE E		82.443	59.429	17.873	1.00 18.28	E
ATOM	5319	СВ	PHE I		81.538				
ATOM						60.108	16.843	1.00 16.99	E
	5320	CG	PHE F		81.905	59.821	15.417	1.00 16.67	E
ATOM	5321		DHE E		82.770	60.661	14.725	1.00 16.72	E
MOTA	5322	CD2	PHE I	122	81.370	58.717	14.756	1.00 17.17	E
ATOM	5323	CE1	PHE E	122	83.096	60.410	13.384	1.00 17.00	E

ATOM	5324	CE2	PHE E	122	81.686	58.456	13.419	1.00 16.82	В
ATOM	5325	CZ	PHE E		82.549	59.305	12.733	1.00 15.81	B
MOTA	5326	c	PHE E		82.287	57.925	17.774	1.00 18.35	E
ATOM	5327	ō	PHE E		83.168	57.231	17.272	1.00 15.90	E
ATOM	5328	N	TYR E		81.157	57.436	18.276	1.00 19.49	E
ATOM	5329	CA	TYR E		80.818	56.021	18.243	1.00 20.92	B
ATOM	5330	СВ	TYR E		81.523	55.261	19.374	1.00 21.02	B
MOTA	5331	CG	TYR E		81.387	53.762	19.247	1.00 20.05	E
ATOM	5332		TYR E		80.242	53.103	19.688	1.00 21.66	В
ATOM	5333		TYR E		80.095	51.726	19.516	1.00 21.85	B
ATOM	5334		TYR E		82.383	53.009	18.633	1.00 20.08	E
ATOM	5335		TYR E		82.250	51.643	18.455	1.00 19.20	B
ATOM	5336	CZ	TYR E		81.105	51.002	18.896	1.00 22,24	E
ATOM	5337	OH	TYR E		80.970	49.640	18.712	1.00 25.26	E
ATOM	5338	C	TYR E		79.311	55.957	18.440	1.00 21.42	B
MOTA	5339	ō	TYR E		78.778	56.647	19.305	1.00 23,90	Б
ATOM	5340	N	PRO E		78.609	55.100	17.676	1.00 20.39	E
ATOM	5341	СD	PRO E		77.155	54.937	17.844	1.00 21.24	E
MOTA	5342	CA	PRO F		79.113	54.177	16.655	1.00 21.61	B
ATOM	5343	СВ	PRO F		77.956	53.188	16.500	1.00 19.35	E
ATOM	5344	CG	PRO E		76.776	54.056	16.670	1.00 19.34	E
MOTA	5345	С	PRO E	124	79.549	54.802	15.325	1.00 20.84	B
ATOM	5346	0	PRO F	124	79.602	56.024	15.184	1.00 22.13	E
ATOM	5347	N	ALA E	125	79.862	53.940	14.361	1.00 22.61	E
MOTA	5348	CA	ALA I	125	80.329	54.341	13.027	1.00 25.48	E
MOTA	5349	CB	ALA I	125	80.860	53.121	12.288	1.00 26.06	E
ATOM	5350	С	ALA I	125	79.311	55.058	12.137	1.00 27.38	B
MOTA	5351	0	ALA I	3 125	79.681	55.906	11.332	1.00 29.08	R
ATOM	5352	N	GLN I	126	78.039	54.706	12.268	1.00 29.18	B
ATOM	5353	CA	GLN F	126	76.990	55.312	11.455	1.00 29.94	E
ATOM	5354	CB	GLN I	3 126	75.625	54.737	11.848	1.00 33.48	B
MOTA	5355	CG	GLN I	3 126	75.536	53.200	11.840	1.00 39.27	E
MOTA	5356	CD	GLN I	3 126	76.067	52.537	13.117	1.00 41.92	E
ATOM	5357		GLW I		77.271	52.523	13.379	1.00 44.02	E
MOTA	5358	NE2	GTM I		75.159	51.981	13.913	1.00 43.83	E
MOTA	5359	C	GLN I		76.977	56.829	11.621	1.00 28.88	E
MOTA	5360	0	GLN I		76.739	57.331	12.719	1.00 28.83	8
MOTA	5361	N		E 127	77.221	57.558	10.532	1.00 27.90	E
ATOM	5362	CA		3 127	77.245	59.018	10.591	1.00 25.67	E
MOTA	5363	СВ		E 127	78.611	59.514	11.150	1.00 25.23	E
MOTA	5364		ILE !		79.693	59.398	10.084	1.00 21.16	E
ATOM	5365	CG1	ILE I		78.504	60.965	11.610	1.00 22.40 1.00 25.35	e
ATOM	5366		ILE I		79.610	61.376 59.673	12.546 9.230	1.00 26.38	E
MOTA	5367	C		E 127	76.985		8.182	1.00 26.20	B
ATOM	5368	0		E 127 E 128	77.196 76.521	59.065 60.916	9.252	1.00 25.64	B
MOTA MOTA	5369 5370	n Ca		B 128	76.248	61.635	8.016	1.00 29.02	E
ATOM	5371	CB		E 128	74.754	61.566	7.671	1.00 29.97	B
ATOM	5372	CG	LYS		74.408	62.178	6.317	1.00 35.17	E
MOTA	5372	CD	_	B 128	75.175	61.487	5.183	1.00 39.63	E
ATOM	5374	CE		E 128	74,936	62.163	3.836	1.00 41.20	B
ATOM	5375	NZ		B 128	75,685	61.492	2.731	1.00 44.74	E
MOTA	5376	C		B 128	76.683	63.090	8.154	1.00 28.40	E
ATOM	5377	ŏ		B 128	76.203	63.812	9.028	1.00 27.15	E
ATOM	5378	N		E 129	77.600	63.506	7.287	1.00 28.99	E
ATOM	5379	CA		B 129	78.119	64.866	7.304	1.00 29.32	E
ATOM	5380	СВ		E 129	79.651	64.860	7.502	1.00 30.69	E
ATOM	5381		VAL		80.171	66.282	7.654	1.00 27.54	E
ATOM	5382		VAL		80.014	64.012	8.721	1.00 30.82	E
ATOM	5383	C		E 129	77.788	65.574	5.992	1.00 30.45	E
ATOM	5384	ō		B 129	78.042	65.039	4.915	1.00 30.36	E
ATOM	5385	N	ARG	E 130	77.221	66.775	6.090	1.00 31.17	E
ATOM	5386	CA	ARG	E 130	76.851	67.562	4.914	1.00 32.17	E
MOTA	5387	CB	ARG	E 130	75.330	67.626	4.764	1.00 34.73	E
MOTA	5388	CG	ARG	E 130	74.632	66.335	4.400	1.00 40.85	E
MOTA	5389	CΦ	ARG	E 130	73.121	66.527	4.511	1.00 46.16	E
ATOM	5390	NE		E 130	72.365	65.456	3.864	1.00 51.33	E
MOTA	5391	\mathbf{cz}		E 130	71.046	65.308	3.959	1.00 53.45	E
ATOM	5392			E 130	70.327	66.162	4.680	1.00 54.21	E
MOTA	5393			B 130	70.444	64.307	3.329	1.00 53.97	E
MOTA	5394	C		E 130	77.359	68.994	5.017	1.00 30.88	E
MOTA	5395	0		E 130	77.321	69.590	6.093	1.00 30.84	E
ATOM	5396	N		E 131	77.831	69.542	3.900	1.00 29.14	E
MOTA	5397	CA	TRP	E 131	78.291	70.928	3.865	1.00 29.57	E

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MOTA	5398	CB	TRP	E	131	79	.538	71	.086	2	. 996	1.0	0 2	27.97	7	В
ATOM	5399	CG	TRP	E	131		. 809		.979		.760			29.37		E
ATOM	5400	CD	2 TRP	E:	131		.342		.949		.671			29.95		E
ATOM	5401	CE	TRP	E:	131		.551		.427		.174			29.75		
ATOM	5402	CE:	TRP	E :	131	80	.913		.209		111			30.39		E
ATOM	5403	CD:	L TRP	B :	131		.689		.941		747			29.02		E
ATOM	5404	NE:	TRP	E:	131		.738		.200		592			0.01		E
ATOM	5405	CZ	TRP	B :	131		.340		.119		.095			8.79		E
ATOM	5406	CZ:					.697		.900		027			1.30		B
ATOM	5407	CH	TRP	E 1	L31		.900		.350		509			1.69		E
ATOM	5408	C	TRP	E 1	L31		.185		.817		301			0.08		E
ATOM	5409	0	TRP	E 1	L31		.449		.413		392					E
ATOM	5410	N	PHE		.32		.081		.027		842			9.15		E
ATOM	5411	CA	PHE				.078		.985		405			9.87		E
ATOM	5412	СB	PHE				.963		.094		443			0.98		E
ATOM	5413	CG	PHE				.041		.918		461			2.09		B
MOTA	5414	CD1	PHE				913		.896		650			3.03 5.25		E
ATOM	5415		PHE				306		.822		273			3.31		E
ATOM	5416		PHE				.055		.794		646					E
ATOM	5417	CE2					460		.717		279			5.49		E
ATOM	5418	\mathbf{cz}	PHE				330		704		461			5.47 5.97		E
ATOM	5419	C	PHE				668		364		182					E
ATOM	5420	0	PHE				537		812		929			2.06 9.15		E
ATOM	5421	N	ARG				186		.026		138					E
ATOM	5422	CA	ARG				613		375		809			4.68 7.78		E
ATOM	5423	CB	ARG				281		420		434			7.78 0.14		E
ATOM	5424	CG	ARG				755		810		005			3.27		E
MOTA	5,425	œ	ARG				474		742	-1.				5.27 6.34		B
ATOM	5426	NE	ARG				096		006	-1.				9.86		E
MOTA	5427	CZ	ARG				441		058	-2.		1.00				E
ATOM	5428	NH1	ARG	B 1	33		124		018	-2.		1.00				E
ATOM	5429		ARG				111		155	-2.		1.00				E
ATOM	5430	C	ARG	E 1	33		343		204		792	1.00				E
ATOM	5431	0	ARG				569		154		835	1.00				B
ATOM	5432	N	ASN				119		940		872	1.00				E
ATOM	5433	CA	asn				941		787		984	1.00				E
ATOM	5434	CB	ASN				040		952		988	1.00				B
ATOM	5435	CG	asn	E 1	34	75.			667		051	1.00				E
MOTA	5436	OD1	ASN	E 1.	34	75.			151		104	1.00				E
MOTA	5437	ND2	ASN	E 1:	34	76.		81.			917	1.00				e
MOTA	5438	C	ASN			72.		79.		2.7		1.00				
ATOM	5439	0	ASN			71.		79.		1.8		1.00				B
ATOM	5440	N	ASP :	E 1:	35	72.		77.		3.5		1.00				E E
MOTA	5441	CA	ASP :	E 13	35	71.		77.		3.4		1.00				E
ATOM	5442	C	ASP :	E 13	35	71.		76.		2.1		1.00				E
ATOM	5443	0	ASP :	E 13	35	70.		75.		1.9		1.00				E
ATOM	5444	N	GLN :	B 13	36	72.	158	76.		1.3		1.00				B
ATOM	5445	CA	GLN :	B 13	36	72.	226	75.		0.1		1.00				E
MOTA	5446	С	GLN I	B 13	36	73.	254	74.		0.3		1.00				e
MOTA	5447	0	GLN :	E 13	36	74.	418	74.		0.6		1.00				B
ATOM	5448	N	GLU 1	E 13	37	72.	829	73.	197	0.1		1.00				E
ATOM	5449	CA	GLU 1	E 13	37	73.	749	72.0	079	0.3	08	1.00				E
MOTA	5450	СВ	GLU 1	B 13	17	72.	992	70.	752	0.4		1.00				E
MOTA	5451	CG	GLU 1			73.5	921	69.	570	0.6	53	1.00				E
MOTA	5452	CD	GLU 1			73.2	210	68.3	334	1.1	66	1.00				E
ATOM	5453		GLU 1			73.9	911	67.3	336	1.4	32	1.00				E
MOTA	5454	OE2	GLU 1			71.9	965	68.3	352	1.3	06	1.00				B
MOTA	5455	C	GLU 1			74.	755	72.0	016	-0.8	33	1.00	47	.37		B
ATOM	5456	0	GLU I	3 13	7	74.3	397	72.:	163	-2.0	00	1.00				E
ATOM	5457		GLU 1			76.0	18	71.8	309	-0.4	77	1.00				B
ATOM	5458		GLU I			77.:	L04	71.7	724	-1.4	44	1.00				E
ATOM	5459		GLU I			78.2		72.6	517	-1.0	11	1.00				2
ATOM	5460		GLU I			77.9	49	74.0	96	-0.9	73	1.00				_ E
ATOM	5461		GLU I			77.9	11	74.7	720	-2.3	54	1.00				B
ATOM	5462		GLU I			78.9		74.6	86	-3.0	44	1.00				E
ATOM	5463		GLU I			76.8	346	75.2	247	-2.7	48	1.00				e
MOTA	5464		GLU I			77.5		70.2	284	-1.5		1.00				_ B
MOTA	5465		GLU E			77.8	198	69.6	65	-0.5		1.00				E
MOTA	5466		THR E			77.6	65	69.7	754	-2.7		1.00				3
MOTA	5467		THR E			78.1	.35	68.3	87	-2.9		1.00				3
MOTA	5468		THR E			77.0	27	67.4	98	-3.5		1.00				3
MOTA	5469		THR E			76.4		68.1	40	-4.7		1.00				3
ATOM	5470		THR E			75.9		67.2		-2.5	25	1.00	48	.03		3
MOTA	5471	C	THR E	13	9	79.3	39	68.4	01	-3.8		1.00				3

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MOTA	5472	0		E 139	80.245	67.574	-3.779	1.00 46.46	В
MOTA	5473	N		E 140	79.339	69.346	-4.827	1.00 46.59	E
ATOM	5474	CA		E 140	80.446			1.00 45.07	E
MOTA MOTA	5475	CB		E 140	79.997			1.00 44.64	E
ATOM	5476 5477	0		B 140 B 140	81.518			1.00 43.57	E
ATOM	5478	N		B 141	81.224		-4.386	1.00 43.33	B
ATOM	5479	CA		E 141	82.756 83.833			1.00 41.31	B
ATOM	5480	c		B 141	84.053		-4.398 -3.034	1.00 38.27 1.00 36.91	E
MOTA	5481	0		E 141	84.930		-2.272	1.00 37.78	e
ATOM	5482	N		3 142	83.245		-2.722	1.00 33.36	E
MOTA	5483	CA		E 142	83.363	68.164	-1.449	1.00 32.16	E
ATOM	5484	CB		3 142	81.978	67.844	-0.847	1.00 31.40	E
ATOM	5485		. VAL 1		82.140	66.995	0.407	1.00 28.96	E
ATOM ATOM	5486 5487		VAL		81.245	69.134	-0.516	1.00 33.20	B
ATOM	5488	0	VAL I		84.140	66.859	-1.576	1.00 31.49	E
ATOM	5489	N	VAL I		83.862 85.118	66.032 66.684	-2.450	1.00 31.67	B
ATOM	5490	CA	VAL I		85.922	65.473	-0.696 -0.675	1.00 30.51 1.00 30.35	E
ATOM	5491	CB	VAL E		87.367	65.731	-1.161	1.00 30.33	E
ATOM	5492	CG1	VAL E		88.096	64.408	-1.348	1.00 32.44	E
MOTA	5493	CG2	VAL E		87.347	66.503	-2.460	1.00 33.96	E
ATOM	5494	C	VAL E		85.966	64.973	0.767	1.00 29.68	E
ATOM	5495	0	VAL E		86.242	65.733	1.695	1.00 29.63	E
ATOM	5496	N	SER E		85.696	63.689	0.946	1.00 28.32	E
ATOM ATOM	5497 5498	CA CB	SER E		85.703	63.090	2.268	1.00 25.38	E
ATOM	5499	OG	SER E		84.295 84.300	62.613 61.845	2.622	1.00 26.70	E
ATOM	5500	C	SER E		86.663	61.916	3.807 2.361	1.00 28.37 1.00 24.56	E
ATOM	5501	ō	SER E		86.824	61.148	1.412	1.00 23.42	e
ATOM	5502	N	THR E		87.320	61.790	3.506	1.00 24.40	B
ATOM	5503	CA	THR E	145	88.218	60.666	3.726	1.00 24.38	E
ATOM	5504	CB	THR E		89.103	60.849	4.983	1.00 24.55	E
ATOM	5505		THR E		88.273	60.815	6.155	1.00 21.59	E
ATOM ATOM	5506		THR E		89.858	62.162	4.935	1.00 24.64	E
ATOM	5507 5508	0	THR E		87.256	59.539	4.055	1.00 23.78	E
ATOM	5509	N	PRO B		86.064 87.745	59.766 58.300	4.242	1.00 23.97	E
ATOM	5510	CD	PRO E		88.993	57.713	4.099 3.585	1.00 25.25 1.00 25.42	E
ATOM	5511	CA	PRO E		86.770	57.264	4.447	1.00 25.42	E
MOTA	5512	CB	PRO E		87.439	55.983	3.951	1.00 26.60	B
ATOM	5513	CG	PRO E	146	88.905	56.293	4.094	1.00 27.24	B
MOTA	5514	C	PRO E		86.597	57.284	5.976	1.00 23.26	E
ATOM	5515	0	PRO B		87.286	58.030	6.672	1.00 21.73	B
ATOM ATOM	5516	N	LEU E		85.669	56.492	6.495	1.00 23.85	E
ATOM	5517 5518	CA CB	TEA E		85.476	56.419	7.936	1.00 23.63	B
ATOM	5519	CG	LEU E		84.355 83.976	55.428	8.260	1.00 25.11	E
ATOM	5520		TER E		83.392	55.241 56.530	9.731 10.270	1.00 28.28 1.00 29.44	E
ATOM	5521		LEU B		82.965	54.116	9.867	1.00 29.44	e
ATOM	5522	C	LEU B		86.812	55.915	8.503	1.00 22.77	B
MOTA	5523	0	LEU E	147	87.366	54.944	8.003	1.00 23.04	E
MOTA	5524	N	ILE E		87.337	56.574	9.530	1.00 21.06	E
ATOM	5525	CA	ITE E		88.614	56.156	10.102	1.00 19.40	E
ATOM	5526	CB	ILE E		89.588	57.355	10.200	1.00 20.05	E
ATOM ATOM	5527 5528		ILE E		90.903	56.922	10.835	1.00 19.93	В
ATOM	5529		IFE E		89.854 90.594	57.918	8.803	1.00 17.58	E
ATOM	5530	c	ILE E		88.449	59.225 55.534	8.821 11.489	1.00 20.23 1.00 17.19	B
MOTA	5531	ō	ILE E		87.820	56.118	12.360	1.00 17.19	E
MOTA	5532	N	ARG E		89.015	54.344	11.677	1.00 15.23	E
ATOM	5533	CA	ARG E	149	88.948	53.638	12.956	1.00 16.42	E
MOTA	5534	CB	ARG E		88.906	52.128	12.724	1.00 20.12	B
ATOM	5535	CG	ARG E		88.903	51.289	14.000	1.00 21.32	E
ATOM	5536	CD	ARG E		88.963	49.802	13.649	1.00 22.44	E
ATOM ATOM	5537 5538	ne Cz	ARG E		87.825	49.382	12.830	1.00 22.55	E
ATOM	5539		ARG E		86.623	49.084	13.313	1.00 22.89	E
MOTA	5540	NH2	ARG E	149	85.650 86.398	48.718 49.139	12.490 14.619	1.00 24.25 1.00 23.36	E
ATOM	5541	С	ARG E		90.174	53.983	13.786	1.00 23.36	B
MOTA	5542	0	ARG E		91.305	53.734	13.363	1.00 16.33	e
MOTA	5543	N	asn e	150	89.953	54.558	14.963	1.00 15.72	E
ATOM	5544	CA	ASN E		91.061	54.948	15.825	1.00 15.93	E
ATOM	5545	CB	asn e	150	90.662 ·	56.125	16.740	1.00 13.37	E

MOTA	5546	CG	ASN E	150	90.278	57.383	15.955	1.00 15.55	E
MOTA	5547		ASN B		90.922	57.739	14.955	1.00 14.20	E
MOTA	5548		ASN E		89.233	58.068	16.414	1.00 15.61	E
MOTA	5549	C	ASN E		91.576	53.786	16.670	1.00 16.79	E
ATOM	5550	ō	ASN B		92.694	53.838	17.180	1.00 18.80	B
ATOM	5551	N		151	90.764	52.745	16.813	1.00 16.63	E
MOTA	5552	CA	GLY E		91.164	51.587	17.593	1.00 18.68	B
ATOM	5553	C	GLY E		90.879	51.684	19.080	1.00 20.19	E
			GLY E		91.087	50.725	19.818	1.00 21.39	E
MOTA	5554	0				52.836	19.539	1.00 19.57	E
MOTA	5555	N	ASP E		90.409		20.954	1.00 19.09	E
MOTA	5556	CA	ASP E		90.108 90.865	52.986	21.531	1.00 18.53	E
ATOM	5557	CB	ASP E		-	54.177		1.00 21.27	E
MOTA	5558	CG	ASP E		90.498	55.481	20.856		E
MOTA	5559		ASP E		89.736	55.453	19.864	1.00 20.11	E
ATOM	5560		ASP E		90.984	56.531	21.321	1.00 22.57	E
MOTA	5561	С	ASP E		88.605	53.156	21.182	1.00 19.23	
ATOM	5562	0	ASP E		88.177	53.840	22.113	1.00 17.78	B
ATOM	5563	N	TRP E		87.816	52.522	20.318	1.00 18.88	E
ATOM	5564	CA	TRP E		86.356	52.566	20.391	1.00 18.61	E
ATOM	5565	CB	TRP E		B5.862	52.162	21.788	1.00 17.06	E
MOTA	5566	CG	TRP E		86.084	50.690	22.085	1.00 17.90	E
MOTA	5567		TRP E		85.165	49.612	21.830	1.00 18.84	E
ATOM	5568		TRP E		85.804	48.414	22.222	1.00 16.88	E
ATOM	5569		TRP E		83.862	49.544	21.308	1.00 18.29	B
MOTA	5570	CD1	TRP E	153	87.209	50.114	22.604	1.00 16.70	B
ATOM	5571	NE1	TRP E	153	87.049	48.747	22.688	1.00 17.49	B
MOTA	5572	CZ2	TRP E	153	85.189	47.164	22.109	1.00 16.54	E
ATOM	5573	CZ3	TRP E	153	83.250	48.303	21.196	1.00 17.19	B
MOTA	5574	CH2	TRP E	153	83.917	47.129	21.597	1.00 17.24	B
ATOM	5575	C	TRP B	153	85.732	53.887	19.975	1.00 18.97	B
ATOM	5576	0	TRP E	153	84.696	54.300	20.508	1.00 18.70	E
MOTA	5577	N	THR E	154	86.378	54.546	19.016	1.00 19.20	E
ATOM	5578	CA	THR E	154	85.876	55.794	18.444	1.00 19.92	B
ATOM	5579	CB	THR E	154	86.442	57.072	19.129	1.00 21.42	E
MOTA	5580	OG1	THR E	154	87.865	57.129	18.958	1.00 19.26	E
ATOM	5581	CG2	THR E	154	86.085	57.096	20.599	1.00 22.17	E
ATOM	5582	C	THR E		86.314	55.835	16.992	1.00 18.66	E
MOTA	5583	0	THR E	154	87.270	55.156	16.603	1.00 19.45	E
ATOM	5584	N	PHE E	155	85.609	56.626	16.193	1.00 18.54	E
ATOM	5585	CA	PHE E		85.940	56.784	14.779	1.00 19.04	E
MOTA	5586	CB	PHE E	155	84.821	56.252	13.882	1.00 20.71	E
ATOM	5587	CG	PHE E		84.524	54.794	14.060	1.00 23.03	E
ATOM	5588		PHE E		83.492	54.375	14.898	1.00 23.94	E
ATOM	5589		PHE E		85.255	53.837	13.365	1.00 23.32	E
ATOM	5590		PHE E		83.189	53.017	15.037	1.00 23.82	E
ATOM	5591		PHE B		84.962	52.476	13.497	1.00 24.46	E
ATOM	5592	CZ	PHE E		83.930	52.068	14.333	1.00 24.51	28
ATOM	5593	C	PHE E		86.109	58.265	14.459	1.00 19.30	B
ATOM	5594	ō	PHE E		85.791	59.134	15.275	1.00 19.12	B
ATOM	5595	N	GLN E		86.613	58.550	13.265	1.00 17.46	B
ATOM	5596	CA	GLN E		86.748	59.924	12.824	1.00 17.87	B
MOTA	5597	CB	GLN E		88.081	60.546	13.264	1.00 19.74	B
ATOM	5598	CG	GLN E		89.330	59.948	12.640	1.00 19.80	E
MOTA	5599	CD	GLN E		90.551	60.785	12.950	1.00 21.46	E
ATOM	5600		GLN E		90.660	61.928	12.503	1.00 21.30	E
ATOM	5601		GLN E		91.469	60.230	13.734	1.00 21.38	E
	5602	C	GLN E		86.629	59.989	11.316	1.00 17.47	B
MOTA	5602	o	GLN E		86.856	58.999	10.616	1.00 17.25	E
MOTA		N	ILE E		86.252	61.159	10.823	1.00 17.46	E
MOTA	5604 5605	CA	ILE E		86.128	61.363	9.397	1.00 18.92	E
MOTA			ILE E		84.746	60.922	8.898	1.00 19.57	E
ATOM	5606		ILE E		83.659	61.774	9.545	1.00 15.09	E
ATOM	5607		. ILE E			60.994	7.369	1.00 21.06	E
MOTA	5608				84.704 83.541	60.334	6.756	1.00 22.57	E
ATOM	5609		ILE E		86.349	62.837	9.083	1.00 20.28	B
MOTA	5610		ILE E		85.887	63.712	9.808	1.00 20.70	E
MOTA	5611		ILE E			63.104	8.019	1.00 20.70	E
MOTA	5612		LEU E		87.094	64.470	7.601	1.00 23.40	B
ATOM	5613		LEU E		87.363 88.869	64.706	7.466	1.00 25.42	E
MOTA	5614		LEU E		89.621	65.141	8.731	1.00 29.38	E
MOTA	5615		LEUE		89.621	64.154	9.864	1.00 27.98	В
MOTA	5616		LEUE		91.118	65.263	8.412	1.00 30.79	B
MOTA	5617		LEU E						E
MOTA	5618		LEU E		86.664	64.736		1.00 23.82	E
ATOM	5619	0	LEU E	728	86.938	100.50	3.204	A.VU &&.00	

T-MOM	5620	N	VAL E 159	85.747	65.702	6.290	1.00 22.98	B
MOTA		CA	VAL E 159	84.990	66.087	5.112	1.00 21.37	E
ATOM	5621		VAL B 159	83.476	66.104	5.417	1.00 20.53	E
MOTA	5622	CB			66.407	4.149	1.00 14.20	E
MOTA	5623		VAL E 159	82.684		6.002	1.00 15.86	8
MOTA	5624		VAL E 159	83.058	64.756		1.00 13.00	E
MOTA	5625	C	VAL E 159	85.468	67.469	4.710	1.00 22.21	E
MOTA	5626	0	VAL B 159	85.253	68.444	5.423		
ATOM	5627	N	MET E 160	86.116	67.539	3.555	1.00 25.37	B
ATOM	5628	CA	MET B 160	86.681	68.779	3.049	1.00 27.07	E
MOTA	5629	CB	MET E 160	88.088	68.494	2.533	1.00 29.57	E
ATOM	5630	CG	MET B 160	88.996	67.954	3.633	1.00 35.17	E
ATOM	5631	SD	MET E 160	90.519	67.185	3.065	1.00 41.54	E
MOTA	5632	CE	MET E 160	90.011	65.462	2.985	1.00 40.10	E
ATOM	5633	C	MET E 160	85.848	69.466	1.979	1.00 28.93	E
ATOM	5634	0	MET E 160	85.191	68.817	1.162	1.00 28.47	E
MOTA	5635	N	LEU E 161	85.875	70.793	1.997	1.00 29.41	E
ATOM	5636	CA	LEU E 161	85,123	71.574	1.031	1.00 31.54	B
ATOM	5637	СВ	LEU E 161	83.931	72.258	1.708	1.00 30.26	E
ATOM	5638	CG	LEU E 161	83.183	73.297	0.860	1.00 30.70	E
ATOM	5639		LEU E 161	82.515	72.618	-0.332	1.00 29.72	E
	5640		LEU E 161	82.145	74.020	1.728	1.00 31.55	E
ATOM			LEU E 161	85.990	72.625	0.363	1.00 32.10	B
MOTA	5641	C	TEO E 191	86.575	73.473	1.029	1.00 32.90	B
MOTA	5642	0		86.063	72.549	-0.960	1.00 35.11	E
ATOM	5643	N	GLU E 162			-1.771	1.00 38.40	E
MOTA	5644	CA	GLU B 162	86.820	73.491		1.00 38.40	E
ATOM	5645	CB	GLU E 162		72.838	-3.105		B
MOTA	5646	CG	GLU E 162		73.776	-4.148	1.00 48.21	E
ATOM	5647	СD	GLU R 162		74.381	-3.711	1.00 52.47	
MOTA	5648	OE1	GLU E 162		73.611	-3.327	1.00 54.02	B
MOTA	5649	OE2	GLU E 162	89.228	75.627	-3.759	1.00 56.21	E
ATOM	5650	C	GLU R 162	85.892	74.673	-2.008	1.00 39.06	E
MOTA	5651	0	GLU E 162	84.750	74.490	-2.422	1.00 39.27	E
ATOM	5652	N	MET E 163	86.369	75.884	-1.747	1.00 40.73	E
ATOM	5653	CA	MET E 163	85.520	77.049	-1.938	1.00 43.18	E
MOTA	5654	CB	MET E 163		77.171	-0.761	1.00 45.15	E
MOTA	5655	CG	MET B 163		76.900	0.612	1.00 47.55	E
ATOM	5656	SD	MET E 163		78.152	1.185	1.00 52.18	B
	5657	CE	MET E 163		79.345	1.941	1.00 50.37	E
MOTA		C	MET E 163		78.371	-2.151	1.00 43.77	E
MOTA	5658		MET E 163		78.477	-1.953	1.00 41.87	E
ATOM	5659	0			79.371	-2.571	1.00 45.83	E
MOTA	5660	N	THR E 164		80.714	-2.827	1.00 49.20	E
MOTA	5661	CA	THR E 164				1.00 50.11	E
ATOM	5662	CB	THR E 164		81.177	-4.241		E
ATOM	5663		THR B 164		80.208	-5.199	1.00 49.28	13
MOTA	5664	CG2			82.535	-4.559	1.00 50.19	
ATOM	5665	C	THR E 164		81.652	-1.785	1.00 51.14	E
ATOM	5666	0	THR B 164		81.916	-1.802	1.00 50.64	B
MOTA	5667	N	PRO E 16		82.170	-0.864	1.00 53.75	B
ATOM	5668	CD	PRO E 16	87.667	82.057	-0.818	1.00 54.65	B
ATOM	5669	CA	PRO E 169	B5.719	83.072	0.185	1.00 56.16	E
ATOM	5670	CB	PRO E 16	86.965	83.299	1.036	1.00 55.47	B
ATOM	5671	CG	PRO E 16	88.057	83.262	0.019	1.00 55.93	E
ATOM	5672	C	PRO E 16	5 85.098	84.381	-0.291	1.00 58.83	E
ATOM	5673	ō	PRO E 16		85.100	-1.112	1.00 58.35	E
ATOM	5674	N	GLN E 16		84.666	0.239	1.00 61.77	E
ATOM	5675	CA	GLN E 16		85.885	-0.065	1.00 63.96	E
ATOM	5676	CB	GLN E 16	_	85.616	-1.123	1.00 64.28	E
ATOM		CG	GLN B 16		85.236	-2.481	1.00 66.42	E
	5677		GLN E 16	_		-3.596	1.00 67.38	E
MOTA	5678			_		-4.761	1.00 68.28	. E
MOTA	5679		1 GLN E 16			-3.244	1.00 66.50	E
MOTA	5680		2 GLN B 16			1.223	1.00 65.40	E
ATOM	5681		GLN E 16			2.007		E
MOTA	5682		GLN E 16				1.00 65.80	E
ATOM	5683		ARG E 16			1.444		E
MOTA	5684					2.647	1.00 65.27	
MOTA	5685					2.706		E
MOTA	5686	CG				4.095		E
MOTA	5687	CD	ARG E 16			5.085		E
MOTA	5688	NE	ARG E 16			6.359		E
MOTA	5689		ARG E 16	7 84.012	90.199	7.394		E
ATOM	5690		1 ARG E 16	7 84.824	89.151	7.318		E
MOTA	5691		2 ARG E 16		90.916	8.509		E
ATOM	5692		ARG E 16			2.684	1.00 63.81	E
MOTA	5693		ARG E 16			1.672	1.00 62.94	B
		-						

MOTA	5694	N	GLY E	168	79.991	87.751	3.860	1.00 61.88	B
MOTA	5695	CA	GLY E	168	78.567	87.519	4.004	1.00 58.78	B
MOTA	5696	c	GLY E		78.243	86.036	3.959	1.00 57.24	E
							4.558	1.00 57.26	B
MOTA	5697	0	GLX E		77.262	85.594			
MOTA	5698	N	ASP E		79.066	85.263	3.249	1.00 54.67	E
MOTA	5699	CA	ASP E	169	78.849	83.823	3.140	1.00 52.07	B
MOTA	5700	CB	ASP E	169	79.799	83.186	2.116	1.00 52.03	Б
ATOM	5701	CG	ASP E		79.329	83.359	0.683	1.00 52.57	B
			ASP E		78.105	83.453	0.457	1.00 51.86	E
ATOM	5702							1.00 52.34	E
MOTA	5703		ASP E		80.188	83.376	-0.223		
MOTA	5704	С	asp e	169	79.027	83.096	4.463	1.00 49.54	E
MOTA	5705	0	ASP E	169	79.993	83.322	5.196	1.00 49.84	E
MOTA	5706	N	VAL E	170	78.082	82.214	4.758	1.00 46.54	E
ATOM	5707	CA	VAL E		78.136	81.418	5.970	1.00 43.15	В
	5708	CB	VAL E		76.903	81.669	6.871	1.00 42.70	E
ATOM								1.00 41.36	B
MOTA	5709		VAL E		76.997	80.819	8.138		
MOTA	5710	CG2	VAL E		76.814	83.146	7.227	1.00 41.14	E
MOTA	5711	C	Val e	170	78.172	79.948	5.555	1.00 41.66	B
MOTA	5712	0	VAL E	170	77.216	79.432	4.972	1.00 40.25	E
ATOM	5713	N	TYR E	171	79.289	79.287	5.833	1.00 39.16	B
ATOM	5714	CA	TYR E		79.438	77.877	5.502	1.00 38.16	E
							4.953	1.00 38.66	E
ATOM	5715	CB	TYR E		80.836	77.617			
MOTA	5716	CG	TYR E		81.035	78.237	3.598	1.00 38.98	E
ATOM	5717	CD1	TYR E	171	80.740	77.522	2.440	1.00 38.79	E
MOTA	5718	CEL	TYR E	171	80.852	78.105	1.186	1.00 40.42	E
ATOM	5719		TYR E		81.451	79.561	3.471	1.00 38.62	B
ATOM	5720	CE2			81.565	80.160	2.219	1.00 40.32	E
					81.262	79.424	1.079	1.00 41.26	R
ATOM	5721	CZ	TYR E						B
MOTA	5722	OH	TYR E		81.350	80.004	-0.166	1.00 42.98	
MOTA	5723	C	TYR E	171	79.206	77.076	6.764	1.00 37.15	R
ATOM	5724	0	TYR E	171	79.755	77.398	7.813	1.00 37.94	E
ATOM	5725	N	THR E	172	78.384	76.037	6.672	1.00 35.12	B
ATOM	5726	CA	THR E		78.091	75.229	7.842	1.00 34.42	E
		CB	THR E		76.654	75.496	8.367	1.00 35.21	B
ATOM	5727						9.094	1.00 35.96	B
MOTA	5728		THR E		76.184	74.351			
ATOM	5729	CG2	THR E	172	75.706	75.790	7.226	1.00 38.35	E
MOTA	5730	C	THR E	172	78.263	73.734	7.638	1.00 32.90	B
MOTA	5731	0	THR E	172	77.875	73.188	6.604	1.00 31.57	E
MOTA	5732	N	CYS E		78.858	73.090	8.643	1.00 30.59	B
ATOM	5733	CA	CYS E		79.078	71.646	8.640	1.00 29.35	E
			CYS E		77.923	71.058	9.454	1.00 29.72	E
MOTA	5734	C						1.00 28.89	E
MOTA	5735	0	CYS E		77.771	71.337	10.645		
MOTA	5736	CB	CYS E	173	80.424	71.299	9.287	1.00 27.53	E
MOTA	5737	SG	CYS E	173	80.875	69.541	9.133	1.00 27.81	E
MOTA	5738	N	HIS E	174	77.109	70.251	8.788	1.00 28.95	E
ATOM	5739	CA	HIS E	174	75.925	69.642	9.381	1.00 28.54	E
MOTA	5740	СВ	HIS E		74.770	69.881	8.399	1.00 29.66	E
			HIS E		73.457	69.311	8.823	1.00 30.98	E
ATOM	5741	CG				69.899	9.369	1.00 31.91	B
ATOM	5742		HIS E		72.367				Ē
MOTA	5743		L HIS E		73.124	67.988	8.630	1.00 31.68	
MOTA	5744	CE	. HIS E	174	71.883	67.785	9.034	1.00 33.26	E
ATOM	5745	NE	HIS E	174	71.401	68.929	9.487	1.00 34.66	E
ATOM	5746	C	HIS E		76.173	68.151	9.650	1.00 27.83	E
ATOM	5747	ō	HIS E		76.438	67.375	8.728	1.00 27.35	B
		N	VAL E		76.085	67.753	10.917	1.00 26.27	E
ATOM	5748					66.365	11.284	1.00 26.34	B
MOTA	5749	CA	VAL E		76.349			1.00 23.90	E
MOTA	5750	CB	VAL I		77.584	66.281	12.215		
MOTA	5751	CG:	L VAL I	3 175	77.807	64.850	12.663	1.00 19.67	B
MOTA	5752	CG:	VAL I	3 175	78.818	66.813	11.491	1.00 19.93	B
MOTA	5753	C	VAL I	3 175	75.199	65.603	11.938	1.00 27.67	E
ATOM	5754	ō	VAL I		74.587	66.064	12.904	1.00 26.77	E
MOTA	5755	N		3 176	74.917	64.423	11.399	1.00 29.83	B
							11.929	1.00 32.99	E
MOTA	5756	CA		3 176	73.864	63.564			Ē
MOTA	5757	CB		B 176	72.842	63.231	10.839	1.00 34.86	
ATOM	5758	CG	GLU 1	E 176	72.076	64.441	10.319	1.00 40.13	E
MOTA	5759	CD	GTD 1	E 176	71.204	64.107	9.124	1.00 44.38	E
ATOM	5760		1 GLU	E 176	70.292	63.265	9.269	1.00 46.31	E
ATOM	5761	OE		E 176	71.433	64.682	8.037	1.00 47.49	E
MOTA	5762	C		B 176	74.526	62.289	12,445	1.00 32.24	E
							11.734	1.00 32.81	E
ATOM	5763	0		E 176	75.296	61.646			E
ATOM	5764	N		E 177	74.220	61.934	13.686	1.00 31.66	
MOTA	5765	CA	HIS	E 177	74.803	60.761	14.311	1.00 30.50	E
MOTA	5766	СВ	HIS	B 177	76.147	61.161	14.927	1.00 29.59	E
ATOM	5767			E 177	76.871	60.034	15.582	1.00 28.23	E

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MOTA	5768	CD2	HIS E	177	77.752	59.134	15.086	1.00 28.22	B
MOTA	5769	ND1	HIS E	177	76.679	59.698	16.903	1.00 27.71	E
			HIS E		77.410	58.636	17.194	1.00 29.83	E
MOTA	5770								
MOTA	5771	NE2	HIS E	177	78.070	58.274	16.108	1.00 29.78	B
MOTA	5772	С	HIS E	177	73.854	60.195	15.373	1.00 30.09	E
MOTA	5773	0	HIS E	177	73.189	60.942	16.083	1.00 29.91	E
MOTA	5774	N	PRO E	7.48	73.781	58.862	15.496	1.00 31.45	B
ATOM	5775	CD	PRO E	178	74.485	57.842	14.697	1.00 31.00	E
ATOM	5776	CA	PRO E	178	72.898	58.226	16.481	1.00 31.44	E
								1.00 30.89	B
MOTA	5777	CB	PRO E		73.370	56.779	16.467		
ATOM	5778	CG	PRO E	178	73.704	56.578	15.028	1.00 31.16	E
ATOM	5779	C	PRO E	178	72.896	58.826	17.893	1.00 31.78	B
						58.727	18.611	1.00 32.84	B
ATOM	5780	0	PRO E		71.903				
ATOM	5781	N	ser e	179	73.996	59.448	18.292	1.00 30.31	B
ATOM	5782	CA	SER E	179	74.087	60.039	19.624	1.00 30.84	E
	5783	CB	SER E		75.552	60.155	20.038	1.00 29.11	B
MOTA						•			
MOTA	5784	OG	ser e	179	76.240	61.049	19.176	1.00 24.79	B
ATOM	5785	С	SER E	179	73.452	61.424	19.717	1.00 32.75	E
MOTA	5786	0	SER E		73.330	61.982	20.804	1.00 32.78	B
								1.00 35.18	В
MOTA	5787	N	LEU E	180	73.046	61.981	18.583		
ATOM	5788	CA	TEO E	180	72.477	63.317	18.578	1.00 37.31	B
MOTA	5789	CB	LEU B	180	73.098	64.132	17.448	1.00 35.77	B
			LEU E		74.610	64.337	17.528	1.00 36.46	B
MOTA	5790	CG							
MOTA	5791	CD1	TEA E	180	75.097	65.018	16.259	1.00 35.16	E
MOTA	5792	CD2	LEU E	180	74.948	65.167	18.752	1.00 34.58	B
		C	LEU E		70.967	63.405	18.463	1.00 40.35	B
MOTA	5793								
ATOM	5794	0	TEO B	180	70.386	63.003	17.456	1.00 40.67	В
MOTA	5795	N	GLN E	181	70.338	63.943	19.503	1.00 42.97	B
ATOM	5796	CA	GLN E	181	68.895	64.141	19.504	1.00 45.09	B
ATOM	5797	CB	GLN E	181	68.466	64.877	20.776	1.00 46.73	B
ATOM	5798	CG	GLN E	181	69.471	65.931	21.235	1.00 49.84	B
MOTA	5799	CD	GLN E	181	68.898	66.904	22.256	1.00 52.17	E
							21.920	1.00 52.91	E
ATOM	5800		GTM E		68.074	67.760			
ATOM	5801	NE2	GLN E	181	69.329	66.774	23.510	1.00 51.73	E
MOTA	5802	С	GLN E	181	68.607	65.002	18.277	1.00 45.26	B
			GLN E		67.660	64.752	17.530	1.00 46.25	E
MOTA	5803	0							
ATOM	5804	N	ser e	182	69.448	66.013	18.078	1.00 44.33	B
ATOM	5805	CA	SER E	182	69.335	66.923	16.943	1.00 42.52	E
MOTA	5806	СВ	SER E		68.819	68.291	17.401	1.00 43.41	E
ATOM	5807	OG	ser e	182	69.658	68.853	18.396	1.00 43.07	E
MOTA	5808	C	ser e	182	70.725	67.068	16.337	1.00 41.70	E
ATOM	5809	0	SER E	182	71.726	66.955	17.040	1.00 39.94	B
						67.330	15.023	1.00 41.57	E
MOTA	5810	N	PRO E		70.805				
MOTA	5811	æ	PRO E	183	69.680	67.554	14.098	1.00 41.72	E
ATOM	5812	CA	PRO E	183	72.087	67.485	14.326	1.00 40.68	E
-			PRO E		71.669	67.638	12.865	1.00 40.95	E
MOTA	5813	CB							
MOTA	5814	CG	PRO E	183	70.344	68.309	12.965	1.00 42.76	E
ATOM	5815	C	PRO E	183	72.988	68.628	14.790	1.00 38.81	E
ATOM	5816	0	PRO E	183	72.520	69.709	15.142	1.00 39.64	B
								1.00 37.31	E
MOTA	5817	И	ILE E		74.291	68.370	14.785		
MOTA	5818	CA	ILE E	184	75.270	69.368	15.177	1.00 34.30	E
ATOM	5819	CB	ILE E	184	76.570	68.728	15.699	1.00 33.43	E
	5820		ILE E		77.671	69.779	15.766	1.00 32.87	E
MOTA									B
MOTA	5821		. ILE E		76.337	68.112	17.076	1.00 33.53	
MOTA	5822	CDI	ILE E	184	77.530	67.339	17.604	1.00 33.29	E
MOTA	5823	С	ILE E	184	75.625	70.216	13.974	1.00 33.68	E
					75.851	69.704	12.882	1.00 33.87	E
MOTA	5824	0	ILE E						
MOTA	5825	N	THR E	185	75.676	71.521	14.181	1.00 34.19	E
MOTA	5826	CA	THR E	185	76.018	72.431	13.111	1.00 33.39	E
MOTA	5827	СВ	THR E		74.792	73.230	12.637	1.00 33.77	E
									E
ATOM	5828		THR E		74.211	73.918	13.751	1.00 33.46	
ATOM	5829	CG2	THR E	185	73.758	72.297	12.016	1.00 33.35	B
ATOM	5830	C	THR E		77.081	73.396	13.590	1.00 33.01	E
					76.990	73.966	14.679	1.00 33.25	E
MOTA	5831	0	THR E						
ATOM	5832	N	VAL E	186	78.106	73.552	12.770	1.00 32.85	E
MOTA	5833	CA	VAL E	186	79.197	74.453	13.067	1.00 32.84	B
ATOM	5834	CB	VAL E		80.503	73.684	13.300	1.00 31.58	E
								1.00 30.07	B
MOTA	5835		I VAL E		81.629	74.651	13.611		
MOTA	5836	CG:	S AYP E	186	80.316	72.697	14.441	1.00 30.84	B
ATOM	5837	C	VAL E		79.329	75.317	11.836	1.00 34.14	B
			VAL E		79.403	74.812	10.719	1.00 33.50	E
ATOM	5838	0						1.00 38.05	E
MOTA	5839	N	GLU E		79.329	76.626	12.029		
ATOM	5840	CA	GLU E	187	79.453	77.522	10.898	1.00 40.60	B
MOTA	5841	CB	GLU E		78.358	78.592	10.934	1.00 43.36	B
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ATOM	5842	CG	GLU !	В	187	78.426	79.531	12.121	1.00 47.46	В
ATOM	5843	CD	GLU :	E	187	77.657	80.822	11.886	1.00 51.49	E
MOTA	5844		GLU			76.452	80.752	11.551	1.00 52.89	B
ATOM	5845		GLU :			78.262	81.908	12.039 10.877	1.00 53.48	E
ATOM ATOM	5846 5847	С 0	GLU :			80.819 81.496	78.182 78.285	11.901	1.00 40.26	E
ATOM	5848	N	TRP			81.221	78.610	9.688	1.00 41.52	E
ATOM	5849	CA	TRP			82,492	79.284	9.488	1.00 43.59	E
MOTA	5850	CB	TRP			83,498	78.337	8.834	1.00 41.24	E
MOTA	5851	CG	TRP	E	188	84.852	78.942	8.675	1.00 41.34	E
MOTA	5852		TRP			85.327	79.672	7.543	1.00 40.23	E
ATOM	5853	CE2			188	86.642	80.090	7.838	1.00 41.87	E
MOTA	5854	CE3	TRP			84.768 85.867	80.015 78.945	6.305 9.588	1.00 40.90	E
ATOM ATOM	5855 5856		TRP			86.947	79.632	9.093	1.00 41.99	B
MOTA	5857	CZ2	TRP			87.411	80.835	6.938	1.00 42.93	E
ATOM	5858	CZ3	TRP			85.531	80.757	5.408	1.00 42.58	E
ATOM	5859	CH2	TRP	B	188	86.839	81.159	5.731	1.00 43.65	B
MOTA	5860	C	TRP		188	82.198	80.467	8.566	1.00 46.04	E
MOTA	5861	0	TRP			81.335	80.374	7.688	1.00 45.30	B
ATOM	5862	N	ARG			82.899 82.673	81.579 82.761	8.765 7.936	1.00 50.26 1.00 54.31	E
MOTA	5863 5864	CA CB	ARG ARG			81.980	83.855	8.755	1.00 56.19	E
ATOM	5865	CG	ARG			82.820	84.460	9.880	1.00 59.58	B
ATOM	5866	CD	ARG			83.030	83.499	11.045	1.00 63.51	E
MOTA	5867	NB	ARG	E	189	83.580	84.180	12.218	1.00 66.73	E
ATOM	5868	CZ	ARG	E	189	84.771	84.771	12.255	1.00 68.44	B
ATOM	5869		ARG			85.553	84.766	11.183	1.00 69.41	E
MOTA	5870		ARG			85.178	85.378	13.363	1.00 70.13	e
ATOM	5871	C	ARG			83.950 85.043	83.322 83.182	7.313 7.866	1.00 55.74 1.00 56.16	E
ATOM ATOM	5872 5873	N N	ALA			83.796	83.962	6.156	1.00 58.53	E
MOTA	5874	CA	ALA			84.920	84.557	5.435	1.00 60.08	E
ATOM	5875	СВ	ALA			84.550	84.734	3.964	1.00 59.97	E
MOTA	5876	C	ALA	E	190	85.335	85.905	6.036	1.00 61.01	B
ATOM	5877	0	ALA			84.654	86.378	6.971	1.00 62.25	E
MOTA	5878		ALA		190	86.338	86.479	5.558	1.00 61.85	E F
MOTA	5879	C	LEU		1	78.718 79.818	38.094 38.571	33.366 33.658	1.00 32.03	F
ATOM ATOM	5880 5881	O N	LEU		1	76.219	38.100	33.307	1.00 33.21	F
MOTA	5882	CA	LEU		ī	77.432	38.678	33.953	1.00 32.59	F
ATOM	5883	N	GLN		2	78.578	37.069	32.531	1.00 30.39	F
ATOM	5884	CA	GLN	F	2	79.744	36.436	31.936	1.00 28.84	F
MOTA	5885	С	GLN		2	79.609	36.081	30.462	1.00 27.93	F
ATOM	5886	0	GLN		2	78.741	35.308	30.067	1.00 27.68	P P
ATOM	5887	N	PRO		3 3	80.463 81.461	36.663 37.720	29.619 29.856	1.00 28.02	F
MOTA MOTA	5888 5889	CD CA	PRO		3	80.370	36.332	28.198	1.00 27.76	F
ATOM	5890	CB	PRO		3	81.363	37.298	27.552	1.00 28.01	F
ATOM	5891	CG	PRO		3	82.353	37.575	28.660	1.00 28.41	F
ATOM	5892	C	PRO	F	3	80.774	34.872	28.030	1.00 27.24	F
MOTA	5893	0	PRO		3	81.698	34.406	28.698	1.00 27.18	F
MOTA	5894	N	PHE		4	80.082	34.144	27.159	1.00 25.22 1.00 24.75	F
ATOM	5895	CA	PHE		4	80.409 79.135	32.738 31.905	26.943 26.849	1.00 25.85	F
ATOM ATOM	5896 5897	CB CG	PHE		4	79.272		27.446	1.00 31.58	F
ATOM	5898		PHE		4	79.435		28.823	1.00 33.24	F
ATOM	5899		PHE		4	79.241	29.404	26.639	1.00 32.15	F
MOTA	5900		PHE			79.561		29.386	1.00 33.28	F
MOTA	5901		PHE			79.364		27.187	1.00 33.29	F
MOTA	5902	CZ	PHE			79.524		28.565 25.664	1.00 34.18	F F
ATOM	5903 5904	C 0	PHE			81.227 80.759		24.586	1.00 24.59	F
MOTA MOTA	5905	N	PRO			82.460		25.771	1.00 22.79	F
ATOM	5906	CD	PRO			83.191		27.029	1.00 21.18	F
MOTA	5907	CA	PRO			83.349	31.882	24.618	1.00 21.18	F
ATOM	5908	СВ	PRO			84.715		25.218	1.00 20.19	F
ATOM	5909	CG	PRO			84.587		26.544	1.00 20.99	F P
MOTA	5910	C	PRO PRO			83.291 82.796		23.949 24.521	1.00 20.28	
MOTA MOTA	5911 5912	И О	GLN			83.818			1.00 21.24	F
MOTA	5913	CA	GLN			83.848			1.00 19.98	
ATOM	5914	СВ	GLN			83.665		20.484	1.00 18.71	
ATOM	5915	CG	GLN	F	6	82.312	30.010	20.048	1.00 18.35	P

MOTA	5916	CD	GLN	F	6	82.255	30.247	18.537	1.00 22.29	F
ATOM	5917		GLN		6	82.612	29.368	17.740	1.00 21.53	F
ATOM	5918		GLN		6	81.802	31.429	18.138	1.00 20.02	F
ATOM	5919	C	GIM		6	85.213	28.548	22.213	1.00 20.47	F
MOTA	5920	0	GLN	P	6	86.243	29.204	22.099	1.00 18.48	F
ATOM	5921	N	PRO	F	7	85.229	27.256	22.575	1.00 21.16	F
ATOM	5922	æ	PRO	F	7	84.071	26.494	23.084	1.00 20.59	F
MOTA	5923	CA	PRO	F	7	86.471	26.520	22.813	1.00 21.61	F
ATOM	5924	CB	PRO	F	7	86.037	25.444	23.797	1.00 23.40	F
MOTA	5925	CG	PRO	F	7	84.649	25.123	23.311	1.00 19.67	F
ATOM	5926	C	PRO	F	7	86.996	25.897	21.521	1.00 23.00	F
MOTA	5927	0	PRO		7	86.219	25.601	20.610	1.00 23.19	F
MOTA	5928	N	GLU		8	88.312	25.714	21.438	1.00 21.78	F
MOTA	5929	CA	GLU		8	88.904	25.068	20.279	1.00 23.12	F
ATOM	5930	CB	GLU		8	90.297	25.632	19.968	1.00 24.50 1.00 26.16	F F
MOTA	5931	CG	GLU		8	91.086 90.360	24.834 24.697	18.915 17.576	1.00 20.10	F
ATOM	5932	CD	GLU		8 8	89.250	24.114	17.540	1.00 33.65	P
MOTA MOTA	5933 5934		GTO		8	90.903	25.171	16.555	1.00 30.66	F
ATOM	5935	C	GLU		8	89.005	23.608	20.680	1,00 22.95	F
ATOM	5936	ō	GTA		8	89.289	23.292	21.833	1.00 23.25	P
ATOM	5937	N	LEU		9	88.756	22.712	19.741	1.00 24.74	F
ATOM	5938	CA	LEU		9	88.815	21.292	20.047	1.00 27.30	P
MOTA	5939	CB	LEU		9	87.729	20.549	19.272	1.00 25.73	F
ATOM	5940	CG	LEU		9	86.302	21.051	19.494	1.00 29.20	F
ATOM	5941	CD1	LEU	F	9	85.338	20.235	18.645	1.00 28.18	P
ATOM	5942	CD2	LEU	F	9	85.938	20.943	20.967	1.00 29.61	F
ATOM	5943	C	LEU	F	9	90.178	20.707	19.712	1.00 28.17	F
ATOM	5944	0	PEA	F	9	90.715	20.940	18.631	1.00 26.94	F
MOTA	5945	N	PRO		10	90.765	19.947	20.647	1.00 30.38	P
ATOM	5946	CD	PRO		10	90.365	19.707	22.044	1.00 30.47	F
ATOM	5947	CA	PRO		10	92.076	19.355	20.370	1.00 34.24	F
ATOM	5948	CB	PRO		10	92.556	18.915	21.752	1.00 32.97 1.00 31.98	F
MOTA	5949	CG	PRO		10	91.282	18.561	22.448 19.393	1.00 35.94	F
MOTA	5950	C	PRO PRO		10 10	91.985 90.993	18.188 17.461	19.376	1.00 38.70	F
ATOM ATOM	5951 5952	o N	TYR		11	93.016	18.031	18.570	1.00 37.40	F
MOTA	5953	CA	TYR		11	93.075	16.936	17.609	1.00 38.84	P
ATOM	5954	CB	TYR		11	92.126	17.176	16.434	1.00 38.73	F
ATOM	5955	CG	TYR		11	92.017	15.969	15.539	1.00 39.56	F
MOTA	5956		TYR		11	91,294	14.848	15.942	1.00 39.88	F
ATOM	5957		TYR		11	91.254	13.697	15.164	1.00 39.49	F
ATOM	5958	CD2	TYR	F	11	92.698	15.913	14.327	1.00 39.73	F
MOTA	5959	CE2	TYR	F	11	92.668	14.765	13.537	1.00 40.44	F
MOTA	5960	CZ	TYR		11	91.945	13.659	13.964	1.00 40.29	F
MOTA	5961	OH	TYR		11	91.921	12.514	13.200	1.00 40.03	F
MOTA	5962	С	TYR		11	94.498	16.781	17.077	1.00 40.23	F F
ATOM	5963	0	TYR		11	95.102	15.708	17.300	1.00 41.88 1.00 40.58	F
MOTA	5964		TYR		11	94.988 37.560	17.742 11.197	16.443 17.272	1.00 17.47	н
MOTA	5965 5966	0	HOH		1 2	81.295	26.543	20.573	1.00 15.95	H
ATOM ATOM	5967	ŏ	нон		3	43.884	23.627	16.726	1.00 14.83	н
ATOM	5968	ŏ	нон		4	89.230	61.015	16.512	1.00 19.10	H
ATOM	5969	ŏ	нон		5	92.090	40.877	18.768	1.00 15.59	H
ATOM	5970	0	HOH		6	57.686	14.054	4.407	1.00 20.02	H
ATOM	5971	0	HOH	н	7	87.607	31.423	22.217	1.00 11.29	H
MOTA	5972	0	HOH		В	31.815	41.479	5.673	1.00 23.91	H
ATOM	5973	0	нон	H	9	46.112	3.594	18.714	1.00 20.15	H
MOTA	5974	0	HOH	H	10	86.724	67.786	15.551	1.00 22.39	. н
MOTA	5975	0	HOH		11	42.599	14.833	17.213	1.00 16.12	H
MOTA	5976	0	HOH		12	93.679	37.081	11.737	1.00 15.03	H
MOTA	5977	0	HOH		13	50.288	0.581	25.262	1.00 13.69	H
MOTA	5978	0	HOH		14	96.256	37.853	25,291	1.00 12.90	H
ATOM	5979	0	HOH		15	90.711	30.936	37.307	1.00 31.88 1.00 33.11	H H
ATOM	5980	0	HOH		16	80.045	39.846	25.144 11.514	1.00 41.56	H
MOTA	5981	0	HOH		17 18	80.708 42.215	45.662 0.119	11.193	1.00 41.56	H
ATOM	5982	0	HOH		18	95.828	50.485	5.930	1.00 27.67	н
MOTA MOTA	5983 5984	Ö	HOH		20	48.809	37.278	14.928	1.00 36.10	H
ATOM	5985	ŏ	HOH		21	47.553	-0.403	11.823	1.00 14.62	H
ATOM	5986	ŏ	HOH		22	94.554	76.132	19.122	1.00 83.80	н
ATOM	5987	ŏ	HOH		23	83.295	48.460	17.328	1.00 17.64	H
ATOM	5988	0	HOF		24	88.976	42.102	7.818	1.00 26.11	H
MOTA	5989	0	HOH		25	99.041	56.322	24.823	1.00 24.86	H

ATOM	5990	0	нон н	26	47.640	0.006	20.312	1.00 18.95	H
ATOM	5991	0	нон н	27	46.987	29.359	11.916	1.00 21.84	H
		ō	нон н	28	88.283	37.229	11.279	1.00 21.34	н
MOTA	5992								
MOTA	5993	0	нон н	29	49.878	-9.043	36.424	1.00 32.47	H
MOTA	5994	0	нон н	30	82.777	39.366	24.935	1.00 24.79	.H
MOTA	5995	0	нон н	31	72.919	25.704	15.123	1.00 18.09	H
MOTA	5996	ō	нон н	32	86.830	25.153	13.558	1.00 24.14	н
MOTA	5997	0	нон н	33	43.152	5.651	13.774	1.00 19.96	н
MOTA	5998	0	нон н	34	100.654	27.732	5.367	1.00 34.73	H
MOTA	5999	0	нон н	35	48.550	32.122	26.894	1.00 20.17	H
			нон н	36	78.728	36.578	6.822	1.00 32.92	н
MOTA	6000	0							
MOTA	6001	0	нон н	37	89.361	11.980	24.953	1.00 51.75	H
MOTA	6002	0	нон н	38	90.411	24.657	31.926	1.00 28,29	H
ATOM	6003	0	нон н	39	80.690	24.233	8.462	1.00 22.43	H
		ō	нон н	40	83.769	65.973	-5.489	1.00 21.06	H
MOTA	6004								
MOTA	6005	0	нон н	41	87.710	34.692	7.008	1.00 22.47	H
ATOM	6006	0	нон н	42	38.997	4.521	15.299	1.00 25.36	H
MOTA	6007	0	нон н	43	94.223	46.644	24.674	1.00 32.67	H
MOTA	6008	o	нон н	44	35.150	15.757	26.294	1.00 29.03	н
MOTA	. 6009	0	нон н	45	85.059	24.652	18.280	1.00 25.63	H
ATOM	6010	0	нон н	46	67.739	6.320	18.991	1.00 43.67	H
MOTA	6011	0	нон н	47	92.376	63.977	12.866	1.00 32.46	H
ATOM	6012	ō	нон н	48	91.526	49.479	22.504	1.00 29.70	H
ATOM	6013	0	нон н	49	56.333	-2.088	24.733	1.00 28.53	H
MOTA	6014	0	нон н	50	100.482	53.937	3.942	1.00 52.26	H
MOTA	6015	0	нон н	51	48.244	18.753	22.918	1.00 44.88	H
ATOM	6016	0	нон н	52	32.577	-0.558	6.769	1,00 33.70	н
			нон н	53	47.162	26.527	12.972	1.00 29.72	н
ATOM	6017	0							
ATOM	6018	0	HOH H	54	98.621	66.834	5.100	1.00 52.20	H
ATOM	6019	0	нон н	55	88.106	52.134	17.293	1.00 21.13	H
ATOM	6020	0	нон н	56	59.655	31.307	17.069	1.00 25.89	H
ATOM	6021	ō	нон н	57	73.562	24.323	12.997	1.00 23.51	H
							20.165	1.00 52.72	H
MOTA	6022	0	нон н	58	43.748	32.725			
ATOM	6023	0	нон н	59	26.392	-7.072	11.400	1.00 26.20	H
ATOM	6024	0	HOH H	60	83.955	73.751	16.805	1.00 18.19	H
ATOM	6025	0	нон н	61	46.229	-19.766	10.675	1.00 28.79	H
MOTA	6026	0	нон н	62	52.436	38.720	16.630	1.00 28.35	H
						9.392	19.914	1.00 28.43	н
MOTA	6027	0	нон н	63	60.555				
ATOM	6028	0	HOH H	64	62.105	2.197	11.948	1.00 33.33	H
ATOM	6029	0	нон н	65	40.514	-12.059	13.631	1.00 21.32	H
MOTA	6030	0	нон н	66	65.876	23.972	14.155	1.00 21.11	н
ATOM	6031	ō	нон н	67	84.702	18.013	5.666	1.00 19.12	H
								1.00 28.72	н
ATOM	6032	0	нон н	68	64.715	11.655	15.936		
MOTA	6033	0	нон н	69	85.418	74.949	14.820	1.00 27.90	H
MOTA	6034	0	нон н	70	77.974	25.419	23.03B	1.00 42.15	H
ATOM	6035	0	нон н	71	65.805	8.484	20.741	1.00 44.01	H
MOTA	6036	ō	нон н	72	51,276	26.045	10.800	1,00 28.36	H
								1.00 36.11	н
ATOM	6037	0	нон н	73	65.226	22.195	25.831		
ATOM	6038	0	нон н	74	101.567	46.068	1.107	1.00 53.81	H
MOTA	6039	0	нон н	75	32.615	31.234	1.517	1.00 21.03	H
MOTA	6040	0	нон н	76	42.100	-0.001	13.802	1.00 23.44	H
ATOM	6041	ō	нон н	77	35.124	40.614	14.668	1.00 27.61	H
		-						1.00 31.64	H
ATOM	6042	0	нон н	78	92.548	46.813	7.595		
ATOM	6043	0	нон н	79	34.670	13.941	14.778	1.00 22.87	H
ATOM	6044	0	нон н	80	98.527	27.671	28.270	1.00 42.07	H
MOTA	6045	0	нон н	81	30.588	36.032	16.540	1.00 37.52	H
				82	89.345	42.957	13.940	1.00 22.73	H
ATOM	6046	0	нон н						
ATOM	6047	0	нон н	83	92.891	18.085	10.698	1.00 32.35	H
ATOM	6048	0	нон н	84	90.050	48.556	16.519	1.00 27.30	н
MOTA	6049	0	HOH H	85	110.812	49.549	15.813	1.00 27.68	H
ATOM	6050	0	нон н	86	75,872	21.668	2.499	1.00 39.37	H
	6051				52.567	14.010	7.270	1.00 34.20	н
ATOM		0	нон н	87					
MOTA	6052	0	нон н	88	69.016	32.569	12.651	1.00 36.96	H
ATOM	6053	0	нон н	89	96.637	25.945	31.742	1.00 37.26	H
ATOM	6054	0	нон н	90	34.496	-12.998	8.560	1.00 22.82	H
MOTA	6055	0	нон н	91	113.021	48.469	17.945	1.00 47.59	H
	6056				34.266	25.052	23.930	1.00 31.02	H
MOTA		0	нон н	92					
MOTA	6057	0	нон н	93	51.464	31.946	19.300	1.00 15.75	Н
MOTA	6058	0	нон н	94	80.054	50.912	15.041	1.00 25.94	H
MOTA	6059	0	нон н	95	40.413	-13.432	16.393	1.00 39.73	H
ATOM	6060	0	нон н	96	57.701	4.191	7.708	1.00 25.27	H
MOTA	6061	ō	нон н	97	80.838	52.853	26.436	1.00 27.67	H
						13.023	20.294	1.00 27.57	H
ATOM	6062	0	нон н	98	58.205				
ATOM	6063	0	нон н	99	41.832	30.497	15.601	1.00 27.32	H

MOTA	6064	0	HOH H 100	72.807	29.880	11.618	1.00 28.05	H
ATOM	6065	0	HOH H 101	48.499	5.079	4.053	1.00 38.72	H
MOTA	6066	0	HOH H 102	100.679	66.408	9.019	1.00 36.21	H
ATOM	6067	0	HOH H 103	45.023	41.442	11.747	1.00 42.72	H
ATOM	6068	ō	HOH H 104	83.296		-2.738	1.00 27.46	
					63.483			н
MOTA	6069	0	HOH H 105	85.067	29.522	34.732	1.00 35.62	H
MOTA	6070	0	HOH H 106	72.272	53.390	15.314	1.00 38.75	H
ATOM			HOH H 107	80.600	27.688	5.225	1.00 26.04	н
	6071	0						
ATOM	6072	0	HOH H 108	71.251	18.567	16.503	1.00 29.08	H
MOTA	6073	0	HOH H 109	88.274	65.356	19.510	1.00 26.70	H
MOTA	6074	0	нон н 110	43.031	4.836	7.813	1.00 38.59	H
ATOM	6075	0	HOH H 111	101.304	35.384	4.755	1.00 43.53	H
MOTA	6076	0	HOH H 112	44.554	10.725	19.619	1.00 21.38	H
ATOM	6077	ō	HOH H 113	115.506	34.478	5.615	1.00 46.62	H
MOTA	6078	0	HOH H 114	36.124	-25.634	9.802	1.00 42.69	H
MOTA	6079	0	HOH H 115	34.494	-33.304	20.170	1.00 61.12	H
ATOM	6080	0	HOH H 116	38.663	26.161	-2.715	1.00 31.39	н
MOTA	6081	0	HOH H 117	105.197	41.384	18.739	1.00 38.53	H
MOTA	6082	0	HOH H 118	38.437	-12.372	18.422	1.00 32.47	H
ATOM	6083	0	HOH H 119	45.430	15.732	9.556	1.00 32.39	н
ATOM	6084	0	HOH H 120	70.475	9.817	-1.029	1.00 53.38	H
MOTA	6085	0	HOH H 121	87.895	64.540	22.445	1.00 47.01	H
MOTA	6086	0	HOH H 122	39.337	36.650	16.644	1.00 25.21	H
MOTA	6087	0	нон н 123	104.091	50.783	20.204	1.00 31.31	H
MOTA	6088	0	HOH H 124	72.528	13.825	20.909	1.00 62.81	H
MOTA	6089	0	HOH H 125	55.353	-5.411	5.747	1.00 25.46	H
MOTA	6090	0	HOH H 126	97.848	63.704	25.177	1.00 27.84	H
MOTA	6091	0	HOH H 127	89.799	75.117	14.074	1.00 49.56	H
MOTA	6092	0	HOH H 128	96.226	35.565	0.211	1.00 40.25	H
							1.00 37.04	H
MOTA	6093	0	HOH H 129		-15.445	19.161		
MOTA	6094	0	HOH H 130	90.627	52.974	9.649	1.00 22.70	H
ATOM	6095	0	HOH H 131	114.398	29.773	11.425	1.00 42.36	H
MOTA	6096	0	HOH H 132	69.810	89.608	-0.164	1.00 53.48	н
MOTA	6097	0	HOH H 133	99.069	30.421	4.728	1.00 31.21	H
MOTA	6098	0	HOH H 134	37.335	49.129	5.746	1.00 43.90	H
MOTA	6099	0	нон н 135	77.753	73.821	17.600	1.00 50.43	H
MOTA	6100	0	нон н 136	44.853	33.208	11.090	1.00 21.26	H
MOTA	6101	0	HOH H 137	88.697	80.608	-4.574	1.00 49.42	H
ATOM	6102	0	HOH H 138	62.018	-6.136	9.010	1.00 30.19	H
ATOM	6103	0	HOH H 139	35.964	-5.810	5.494	1.00 45.47	H
MOTA	6104	0	HOH H 140	73.968	65.480	8.013	1.00 43.93	H
ATOM	6105	0	HOH H 141	78.361	66.868	24.455	1.00 57.76	H
	6106		HOH H 142	53.527	3.199	22.332	1.00 32.95	н
MOTA		0						
MOTA	6107	0	HOH H 143	56.018	-6.530	25.205	1.00 42.75	н
ATOM	6108	0	HOH H 144	82,930	52.617	28.345	1.00 32.35	н
MOTA	6109	o	HOH H 145		-21.313	24.210	1.00 48.87	H
MOTA	6110	0	HOH H 146	86.079	41.197	35.698	1.00 36.97	H
ATOM	6111	0	HOH H 147	35.017	8.399	11.516	1.00 32.21	H
ATOM	6112	0	HOH H 148	25.864	-19.905	17.166	1.00 41.53	H
MOTA	6113	0	нон н 149	55.504	20.659	6.959	1.00 36.63	H
MOTA	6114	0	HOH H 150	106.046	47.260	19.571	1.00 30.60	H
ATOM	6115	0	HOH H 151	108.769	26.147	5.447	1.00 48.82	н
MOTA	6116	0	нон н 152	38.689	17.576	4.331	1.00 39.07	H
MOTA	6117	0	HOH H 153	97.787	62.580	8.740	1.00 29.61	H
ATOM	6118	0	HOH H 154	59,501	-12.817	20.769	1.00 50.36	H
ATOM	6119	0	HOH H 155	47.887	40.072	-4.641	1.00 51.05	H
MOTA	6120	0	HOH H 156	60.057	16.564	27.477	1.00 40.66	H
MOTA	6121	0	HOH H 157	67.048	27.841	20.873	1.00 39.66	H
ATOM	6122	0	HOH H 158	37.028	32.932	18.669	1.00 37.23	H
							1.00 46.64	
MOTA	6123	0	нон н 159	121.780	18.693	-3.076		н
MOTA	6124	0	HOH H 160	39,196	18.091	27.271	1.00 29.99	H
MOTA	6125	0	HOH H 161	113.285	44.237	19.561	1.00 39.04	H
MOTA	6126	ō	HOH H 162	43.379		19.370	1.00 27.58	H
MOTA	6127	0	HOH H 163	91.636		11.885	1.00 54.73	H
MOTA	6128	0	HOH H 164	113.381	46.844	20.020	1.00 54.22	H
ATOM	6129	ō	HOH H 165	79.238		24.112	1.00 36.07	H
ATOM	6130	0	HOH H 166	27.985		18.424	1.00 36.25	н
ATOM	6131	0	нон н 167	34.709	-10.661	20.615	1.00 9.89	H
MOTA	6132	0	HOH H 168	93.577	37.339	20.182	1.00 14.03	н
								H
MOTA	6133	0	нон н 169	97.912		7.309	1.00 24.22	
ATOM	6134	0	HOH H 170	69.616	4.375	18.521	1.00 38.01	H
MOTA	6135	0	нон н 171	80.870	25.194	6.002	1.00 21.84	H
				50.564		5.906	1.00 32.25	н
mota Mota	6136 6137	0	HOH H 172 HOH H 173	88.207		13.919	1.00 19.68	H

ATOM	6138	0	HOH H 174	93.800	47.651	27.174	1.00 41.65	H
ATOM	6139	0	HOH H 175	52.842	0.304	25.210	1.00 28.07	H
ATOM	6140	0	HOH H 176	66.457	4.742	14.051	1.00 28.64	H
ATOM	6141	ō	HOH H 177	36.948	12.416	15.109	1.00 28.66	н
ATOM	6142	ŏ	HOH H 178	103.292	41.793	7.607	1.00 28.51	н
			HOH H 179				1.00 27.43	
MOTA	6143	0		86.476	36.035	9.339		H
MOTA	6144	0	HOH H 180	82.262	41.159	26.845	1.00 24.13	H
ATOM	6145	0	HOH H 181	32.348	15.030	26.400	1.00 30.06	H
MOTA	6146	0	HOH H 182	69.916	30.709	14.482	1.00 42.81	H
ATOM	6147	0	HOH H 183	48.060	10.142	26.751	1.00 49.12	н
ATOM	6148	0	HOH H 184	45.863	-9.131	37.252	1.00 43.70	н
ATOM	6149	ō	HOH H 185	32.095	-3.806	34.251	1.00 41.46	н
MOTA	6150	ō	HOH H 186	108.258	31.975	8.914	1.00 33.62	н
					64.293		1.00 54.43	н
ATOM	6151	0	HOH H 187	99.465		8.210		
MOTA	6152	0	нон н 188	74.677	30.785	27.841	1.00 28.20	H
MOTA	6153	0	HOH H 189	44.953	0.968	35.892	1.00 32.25	Н
ATOM	6154	0	HOH H 190	88.523	27.792	36.268	1.00 30.83	H
MOTA	6155	0	HOH H 191	37.736	8.611	11.729	1.00 38.92	H
MOTA	6156	0	HOH H 192	35.988	45.178	12.964	1.00 33.85	H
ATOM	6157	0	HOH H 193	77.222	68.027	1.401	1.00 27.02	н
ATOM	6158	0	HOH H 194	63.326	-8.764	15.926	1.00 38.46	H
ATOM	6159	ō	нон н 195	109.635	61.489	27.644	1.00 52.79	H
ATOM	6160	ō	нон н 196	101.299	67.528	11.319	1.00 38.92	H
ATOM	6161	0	нон н 197	77.295	56.116	25.768	1.00 36.83	н
ATOM	6162	0	HOH H 198	81.538	22.288	0.320	1.00 47.08	H
ATOM	6163	0	HOH H 199	55.989	3.900	0.756	1.00 46.35	H
MOTA	6164	0	HOH H 200	66.200	40.514	17.513	1.00 43.54	H
MOTA	6165	0	HOH H 201	40.497	-1.046	9.238	1.00 27.84	H
ATOM	6166	0	HOH H 202	57.171	27.504	8.258	1.00 52.74	H
ATOM	6167	0	нон н 203	44.592	-6.430	37.531	1.00 37.55	H
ATOM	6168	ō	HOH H 204	26.892	-1.642	9.494	1.00 55.58	Н
ATOM	6169	ŏ	нон н 205	83.350	58.389	2.759	1.00 46.24	н
				112.353	45.284	9.770	1.00 30.99	H
ATOM	6170	0	нон н 206					
ATOM	6171	0	нон н 207	86.315	23.927	16.100	1.00 41.36	H
ATOM	6172	0	HOH H 208	67.053	45.396	12.396	1.00 31.02	н
ATOM	6173	0	HOH H 209	111.609	60.418	8.362	1.00 52.01	H
ATOM	6174	0	HOH H 210	91.254	47.553	32.752	1.00 41.71	H
MOTA	6175	0	HOH H 211	88.489	39.944	11.117	1.00 34.00	H
ATOM	6176	0	HOH H 212	104.972	69.233	16.415	1.00 37.26	H
ATOM	6177	o	HOH H 213	23.462	39.893	6.692	1.00 56.45	H
MOTA	6178	ŏ	HOH H 214	84.114	54.447	-1.718	1.00 42.58	н
ATOM	6179	ō	HOH H 215	105.045	66.068	22.775	1.00 24.48	н
			нон н 216	85.378	52.388	17.025	1.00 37.91	н
ATOM	6180	0						H
MOTA	6181	0	нон н 217	91.411	30.837	4.259	1.00 23.59	
ATOM	6182	0	HOH H 218	99.019	37.803	25.178	1.00 37.20	H
ATOM	6183	0	HOH H 219	88.866	41.183	35.781	1.00 42.88	H
MOTA	6184	0	нон н 220	66.946	25.931	12.530	1.00 45.53	H
MOTA	6185	0	HOH H 221	83.809	61.544	-0.645	1.00 32.51	н
ATOM	6186	0	HOH H 222	91.766	28.386	3.286	1.00 29.97	H
ATOM	6187	0	HOH H 223	83.302	45.674	11.423	1.00 40.65	H
ATOM	6188	ō	HOH H 224	59.198	3.628	18.904	1.00 22.61	H
ATOM	6189	ō	нон н 225		-11.852	5.930	1.00 29.77	H
	6190		нон н 226	88.953	22.712	24.560	1.00 23.54	н
ATOM		0		108.379	54.102	21.160	1.00 23.34	н
MOTA	6191	0	HOH H 227					
ATOM	6192	0	нон н 228	44.957	16.820	6.827	1.00 37.14	н
MOTA	6193	0	нон н 229	105.872	50.217	22.393	1.00 33.77	H
ATOM	6194	0	HOH H 230	40.390	52.287	-1.729	1.00 62.00	H
ATOM	6195	0	HOH H 231	103.837	27.586	24.806	1.00 50.76	H
ATOM	6196	0	HOH H 232	50.931	9.397	25.207	1.00 40.65	H
ATOM	6197	0	нон н 233	64.739	2.382	27.973	1.00 46.98	· H
ATOM	6198	ō	HOH H 234	38.363	0.460	8.402	1.00 28.58	H
ATOM	6199	ŏ	нон н 235	73.577	50.129	18.561	1.00 36.68	н
ATOM	6200	٥	HOH H 236	100.912	58.519	6.876	1.00 36.99	н
				100.512	26.841	26.380	1.00 36.27	H
ATOM	6201	0	нон н 237					н
MOTA	6202	0	нон н 238	82,528	48.080	12.484	1.00 44.97	
MOTA	6203	0	нон н 239	70.870	44.782	13.746	1.00 26.53	H
MOTA	6204	0	HOH H 240	71.914	-9.049	17.302	1.00 59.29	H
ATOM	6205	0	HOH H 241	28.024	9.146	32.377	1.00 43.91	H
MOTA	6206	0	HOH H 242	55.531	-2.470	4.880	1.00 50.20	Н
MOTA	6207	0	HOH H 243	63.362	16.623	21.334	1.00 30.95	H
ATOM	6208	ō	HOH H 244	71.813	27.548	12.914	1.00 54.77	H
MOTA	6209	ŏ	HOH H 245	22.793	-3.930	12.731	1.00 39.10	н
ATOM	6210	o	HOH H 246	73.087	44.091	34.124	1.00 47.86	H
ATOM				48.717	31.774	19.850	1.00 33.46	н
TA OM	6211	0	HOH H 247	40.141	32.1/4	LD. 000	4.00 33.40	••

MOTA	6212	0	HOH H 248	100.851	61.218	7.741	1,00 35.49	н
MOTA	6213	0	HOH H 249	116.291	47.311	12.227	1.00 49.67	H
MOTA	6214	0	HOH H 250	99.469	40.748	22.418	1.00 25.82	H
ATOM	6215	0	HOH H 251	52.271	4.031	24.614	1.00 44.68	H
MOTA	6216	0	HOH H 252	106.629	40.298	32.271	1.00 59.44	н
MOTA	6217	0	нон н 253	45.587	-9.303	3.049	1.00 26.81	H
MOTA	6218	0	HOH H 254	52.547	-9.432	27.670	1.00 45.08	H
MOTA	6219	0	HOH H 255	75.854	21.157	27.640	1.00 42.33 1.00 37.84	H
MOTA	6220	0	HOH H 256	82.119	63.444	23.430 18.936	1.00 37.84	H H
MOTA	6221	0	HOH H 257 HOH H 258	104.091 79.477	38.660 56.121	8.190	1.00 30.23	н
MOTA MOTA	6222 6223	o	HOH H 259	101.351	32.257	5.631	1.00 29.94	H
MOTA	6224	ŏ	нон н 260	93.989	23.313	31.488	1.00 35.30	H
ATOM	6225	ō	HOH H 261	28.754	-1.723	6.977	1.00 36.90	H
ATOM	6226	ō	HOH H 262	93.007	48.370	9.901	1.00 49.06	H
MOTA	6227	0	нон н 263	82,990	88.137	9.529	1.00 39.70	н
MOTA	6228	0	HOH H 264	118.031	51.582	0.542	1.00 36.21	H
ATOM	6229	0	HOH H 265	21.682	15.046	11.602	1.00 62.29	н
MOTA	6230	0	нон н 266	34.210	24.576	5.314	1.00 18.89	H
MOTA	6231	0	нон н 267	85.829	40.095	14.911	1.00 25.26	H
ATOM	6232	0	нон н 268	102.070	38.308	21.059	1.00 41.79	H
MOTA	6233	0	нон н 269	41.071	-2.346	7.039	1.00 38.87	H H
ATOM	6234	0	нон н 270 нон н 271	68.717	3.686 -12.649	16.083 12.753	1.00 37.79 1.00 29.26	н
MOTA	6235	0	HOH H 271	36.426	24.744	4.145	1.00 45.88	H
ATOM ATOM	6236 6237	0	HOH H 272	88.670	31.858	5.525	1.00 39.43	H
ATOM	6238	Ö	HOH H 274	90.819	38.524	36.028	1.00 30.15	н
ATOM	6239	ŏ	нон н 275	90.790	49.861	10.317	1.00 39.97	н
ATOM	6240	0	HOH H 276	77.026	11.969	13.970	1.00 44.87	H
ATOM	6241	0	нон н 277	36.555	12.078	12.344	1.00 40.47	H
ATOM	6242	0	HOH H 278	52.331	7.302	24.972	1.00 49.30	н
MOTA	6243	0	нон н 279	92.612	33.229	3.564	1.00 40.55	Н
ATOM	6244	0	HOH H 280	83.546	64.142	25.612	1.00 50.28	н
ATOM	6245	0	HOH H 281	28.206	-1.891	36.868	1.00 44.06	H
MOTA	6246	0	HOH H 282	93.185	20.914 41.763	30.917 24.500	1.00 44.51 1.00 44.20	н
ATOM	6247	0	HOH H 283 HOH H 284	98.176 29.174	-0.123	4.304	1.00 46.75	н
MOTA MOTA	6248 6249	o	HOH H 285	79.206	77.643	14.919	1.00 30.21	Н
ATOM	6250	ŏ	нон н 286	90.531	26.085	37.436	1.00 36.96	н
ATOM	6251	ō	нон н 287	55.726	0.396	21.054	1.00 49.55	H
MOTA	6252	0	HOH H 288	111.246	30.915	19.699	1.00 42.91	H
MOTA	6253	0	HOH H 289	77.000	58.921	5.300	1.00 47.04	H
ATOM	6254	Ο,	нон н 290	34.339	-9.458	5.288	1.00 25.50	H
MOTA	6255	0	HOH H 291	109.784	29.168	15.534 29.650	1.00 45.96 1.00 48.76	H H
ATOM	6256	0	нон н 292 нон н 293	93.674 92.299	48.853 47.066	3.801	1.00 37.41	н
MOTA MOTA	6257 6258	Ö	HOH H 294	110.965	23.141	11.799	1.00 42.97	н
ATOM	6259	ŏ	HOH H 295	90.562	45.235	33.919	1.00 33.83	н
ATOM	6260	ō	HOH H 296		-10.500	25.018	1.00 49.78	H
MOTA	6261	ō	нон н 297	54.676	36.195	11.362	1.00 54.22	H
MOTA	6262	0	HOH H 298	107.263	59.234	5.282	1.00 56.05	H
MOTA	6263	0	нон н 299	70.560	48.918	1.476	1.00 49.72	Н
MOTA.	6264	0	нон н зоо	84.037	38.916	5.971	1.00 39.33	H
MOTA	6265	0	HOH H 301	86.468	41.381	11.971	1.00 45.69	H
ATOM	6266	0	нон н 302	24.400	11.569	23.610	1.00 36.73 1.00 46.20	H
ATOM	6267	0	HOH H 303	73.087 72.681	79.808 43.116	7.028 14.941	1.00 40.20	н
ATOM	6268	0	HOH H 304 HOH H 305	84.844	42.198	15.611	1.00 26.23	н
ATOM ATOM	6269 6270	0	нон н 306	54.135	19.007	24.978	1.00 27.41	H
ATOM	6271	ŏ	нон н 307	67.044	10.459	18.465	1.00 44.92	н
ATOM	6272	ō	HOH H 308	82.262	49,436	14.864	1.00 39.04	. н
ATOM	6273	0	нон н 309	114.093	50.994	16.895	1.00 43.32	H
MOTA	6274	0	нон н 310	64.428	3.092	30.590	1.00 43.29	H
MOTA	6275	0	HOH H 311	81.152	70.187	18.656	1.00 34.21	H
MOTA	6276	0	нон н 312	74.596	81.584	-2.515	1.00 55.00	H
MOTA	6277	0	нон н 313	61.161	25.774	22.464	1.00 32.98	H
MOTA	6278	0	HOH H 314	53.149	-7.019	4.754 33.567	1.00 26.01 1.00 40.32	H H
MOTA	6279	0	нон н 315 нон н 316	44.571 82.293	8.317 49.769	10.587		н
MOTA MOTA	6280 6281	0	HOH H 317	48.467	8.859	24.614	1.00 42.38	н
MOTA	6282	Ö	нон н 317	56.588		4.728	1.00 44.65	н
MOTA	6283	ŏ	нон н 319		-23.239	26.551	1.00 42.45	H
ATOM	6284	0	нон н 320	82.483		7.719	1.00 39.22	H
ATOM	6285	0	HOH H 321	82.063	19.937	23.440	1.00 35.69	н

106.025 63.366 22.616 1.00 31.93 ATOM 6286 HOH H 322 H 9.890 8.669 1.00 38.11 H ATOM 6287 0 HOH H 323 46,181 75.56B 6.998 1.00 41.82 ATOM 6288 ٥ HOH H 324 71.708 H ATOM 6289 ٥ HOH H 325 108.280 34.405 3.851 1.00 30.72 н 1.00 40.72 MOTA 6290 0 HOH H 326 32,275 40.921 14.635 H 37.556 15.785 5.690 1.00 42.29 Н 6291 0 ATOM HOH H 327 37.182 1.00 31.78 н MOTA 6292 0 HOH H 328 85.569 33.598 6293 0 HOH H 329 33.070 -11.287 23.137 1.00 48.90 H ATOM 6294 HOH H 330 87.593 16.513 19.683 1.00 45.53 ATOM 0 H HOH H 331 53.631 17.853 1.00 39.81 MOTA 6295 0 116,176 ATOM 6296 ٥ HOH H 332 26.940 -11.377 14.930 1.00 39.40 H 60.033 22.456 1.00 32.84 H MOTA 6297 0 нон н ззз 28.679 HOH H 334 52.472 15.182 2.562 1.00 48.72 н MOTA 6298 0 1.00 40.99 Н 84.377 54.588 4.646 ATOM 6299 0 HOH H 335 115.759 67.454 19.970 1.00 46,15 H ATOM 6300 HOH H 336 H MOTA 6301 0 HOH H 337 88.969 52.684 25.112 1.00 42.31 36.351 12.852 9.875 1.00 37.11 0 HOH H 338 ATOM 6302 1.00 49.82 H MOTA 6303 ٥ HOH H 339 97.702 31.578 2.653 6304 0 HOH H 340 53.964 -6.543 26.981 1.00 35.52 H ATOM ATOM 6305 0 HOH H 341 24.475 -17.438 17.094 1.00 38.04 Н 58.530 0.915 19.036 1.00 43.08 H 0 HOH H 342 6306 ATOM 39.025 н 77.156 37.203 1.00 48.54 ATOM 6307 0 HOH H 343 Н ATOM 6308 HOH H 344 49.978 -1.361 0.435 1.00 39.48 6309 0 HOH H 345 53.900 37.104 13.703 1.00 47.74 н ATOM 13.575 1.00 57.13 H HOH H 346 77.886 49.625 ATOM 6310 0 Н 0.570 1.00 50.38 MOTA 6311 0 HOH H 347 57.053 8.721 ATOM 6312 0 HOH H 348 96.803 63.745 10.854 1.00 41.14 Н Н 89.009 70.808 11.906 1.00 45.67 6313 0 HOH H 349 ATOM 8.221 1.00 42.47 н 22.353 66.363 ATOM 6314 0 HOH H 350 н 6315 0 HOH H 351 52.578 25.044 8.541 1.00 41.16 ATOM 81.789 73.640 -3.536 1.00 50.48 н MOTA 6316 HOH H 352 Н 67.632 -11.181 13.891 1.00 48.24 MOTA 6317 0 HOH H 353 22.367 1.00 14.47 41.357 -5.652 ATOM 6318 0 HOH H 354 G 6319 C1 EDO G 501 37,685 -5.096 30.876 1.00 23.96 ATOM G 38.224 -4.213 31.883 1.00 23.38 MOTA 6320 01 EDO G 501 EDO G 501 38.742 -6.046 30.406 1.00 25.29 G 6321 C2 ATOM G 39.062 -6.931 31.464 1.00 26.30 EDO G 501 ATOM 6322 02 1.00 41.69 89.146 26.377 27.000 MOTA 6323 C1 EDO G 502 G EDO G 502 88.631 26.508 28.343 1.00 51.10 MOTA 6324 01 26.303 1.00 43.14 G EDO G 502 88.436 25,261 ATOM 6325 C2 88,726 24.052 26.967 1,00 41,73 MOTA 6326 02 EDO G 502 1.00 21.00 G 30.633 6327 C1 **EDO G 503** 85.093 31,920 ATOM 85.283 30.597 G ATOM 6328 01 **EDO G 503** 31.203 1.00 18.65 1.00 19.69 31.186 G C2 EDO G 503 83.846 32.561 6329 MOTA 84.148 33.101 32.454 1.00 20.94 G EDO G 503 ATOM 6330 02 1.00 38.01 25.885 34.956 3.907 MOTA 6331 C1 **EDO G 504** G 1.00 36.69 EDO.G 504 33.976 2.838 25.869 ATOM 6332 01 EDO G 504 36.360 3.344 25.982 1.00 39.84 G MOTA 6333 C2 36.573 2.396 24.935 1.00 33.51 **EDO G 504** ATOM 6334 02 END

Example 4

Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition (IC $_{50}$) is calculated. Since the level of IC $_{50}$ may vary between separate titration experiments, the IC $_{50}$ values are compared to the IC $_{50}$ of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: IC $_{50}$ of reference peptide / IC $_{50}$ of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the β -subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of IC $_{50}$. A peptide analog with an IC $_{50}$ value of less than 100 μ M is suitable for further screenings.

[92] Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β-subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of IC₅₀ or K_i.

Candidate peptide analogs are further tested for their ability to inhibit proliferation of [93] T cells specific for gluten peptides. This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X 10⁴ TCC with 5 X 10⁴ fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [3H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 μM or greater are suitable for further screening.

[94] All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95] Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

1. An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

- The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises
 one or more naturally occurring amino acids, non-naturally occurring amino acids, modified
 amino acids, or amino acid mimetics.
- 3. The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
- 4. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.
- 5. The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.
- [96] 6. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.
 - 7. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.
 - 8. The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
 - 9. The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence $PFPQX_1ELX_2Y$, where X_1 and X_2 are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of X_1 and X_2 is a residue other than proline

10. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

- 11. The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.
- 12. A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:

administering to a patient an effective dose of an HLA-binding peptide inhibitor; wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

- 13. The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.
- 14. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.
- 15. The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.
- 16. A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:

an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

- 17. The formulation according to Claim 16, further comprising an enteric coating.
- 18. Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.
- 19. A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
- a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

- a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said threedimensional representation; and
- a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 20. A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
- (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;
- (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
- (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.